

08-14-00

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BOX SER

PATENT

Attorney Docket No: UCAL-246/02/1US  
96-026-5

Express Mail Label Number: EL514038279US  
Date of Deposit: August 10, 2000

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Date:

10 August 2000

By:

*Vladimir Skliba*

Vladimir Skliba

Box Patent Application  
Assistant Commissioner for Patents  
Washington, D.C. 20231

NEW PATENT APPLICATION TRANSMITTAL

1. Transmitted herewith for filing is a:
  - a. ☒ utility patent application
  - b. Inventor(s): BAXTER, John D.; FLETTERICK; Robert J.; and KUSHNER, Peter J.
  - c. For: NUCLEAR RECEPTOR LIGANDS AND LIGAND BINDING DOMAINS
2. Enclosed are:
  - a. ☒ 50 sheets of informal sheets of drawings.
  - b. ☒ Letter to Official Draftsperson replacing the informal sheets of drawings with the following sheets of Formal Drawings:
    1. 12 sheets of black and white photographs
    2. 3 sets of the four color photographs, i.e. 12 sheets of color photographs,
    3. 34 sheets of black and white drawings
  - c. ☒ Petition to Accept Color Photographs

- d. ☒ A copy of executed Declaration(s) and Power(s) of Attorney as filed in parent application Serial No. 08/980,115, filed November 26, 1997.
- e. ☒ Statement Verifying the Identity of Computer Readable and Paper Copies of Sequence Listing.
- f. ☒ Preliminary Amendment (also entering SEQ ID NOs where the description or claims discuss a listed sequence, in accordance with 37 CFR §1.821(d).
- g. ☒ Request to Delete Names of Persons who are not Inventors.

3. This application is a:

☒ divisional application of U.S. Application Serial No.08/980,115, filed November 26, 1997.

The filing fee has been calculated as shown below:

☒ Utility application:

CLAIMS AFTER ENTRY OF ANY AMENDMENTS, LESS ANY CANCELLED CLAIMS

FOR:	Claims Filed			Extra Claims <sup>1</sup>	Small Entity Rate Fee		Other Than a Small Entity Rate Fee		Total Filing Fee
Basic Fee					\$345		\$690		\$690.00
Total Claims	4	-20=	0		\$9		\$18		\$0.00
Independent Claims	4	-3=	1		\$39		\$78		\$78.00
Multiple Dependent Claims Presented					\$130		\$260		\$0.00
TOTAL									\$768.00

<sup>1</sup> If difference is negative, enter "0".

☒ Petition to Accept Color Photographs (\$130.00) .....\$130.00

**TOTAL FEES: .....\$898.00**

☒ A check for the amount of the above indicated TOTAL FEES is attached.



Conditional Petition for Extension of Time: An extension of time is requested to provide for timely filing if an extension of time is still required after all papers filed with this transmittal have been considered.

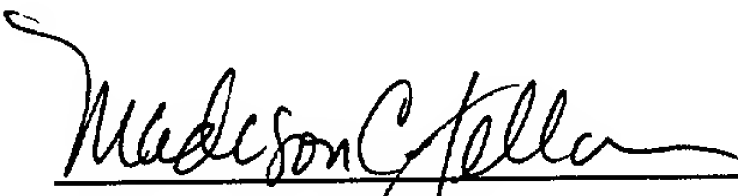
The Commissioner is hereby authorized to charge any underpayment of the following fees associated with this communication, or credit any overpayment to Deposit Account No. 03-3117:

- ☒ Any national application filing fees under 37 CFR 1.16.
- ☒ Any patent application processing fees under 37 CFR 1.17.

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Respectfully submitted,  
COOLEY GODWARD LLP

By:

  
\_\_\_\_\_  
Madison C. Jellins  
Reg. No. 35,555

Attorney Docket No: UCAL-246/02/1US  
96-026-5

PATENT

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Date: 10 August 2000 By: Vladimir Skliba  
Vladimir Skliba

**IN THE UNITED STATES PATENT AND TRADEMARK OFFICE**

In re application of BAXTER, John D. et al.

Serial No.: Not yet assigned Examiner: Not yet assigned  
Filed: August 10, 2000 Art Unit: Not yet assigned  
For: NUCLEAR RECEPTOR LIGANDS AND LIGAND BINDING DOMAINS

BOX PATENT APPLICATION  
Commissioner for Patents  
Washington, D.C. 20231

**PRELIMINARY AMENDMENT**

Prior to examination of the above-identified application, the Examiner is respectfully requested to enter the following amendments.

IN THE SPECIFICATION

On Page 1, please delete the following:

"ACKNOWLEDGMENTS

This invention was supported in part by grants from the National Institutes of Health grant number 1 R01 DK43787, and 5 R01 DK 41842. The U.S. Government may have rights in this invention.

### CROSS-REFERENCE TO RELATED APPLICATIONS

This application claims the benefit of the following provisional applications: United States Ser. No. 60/008,540 and 60/008,543, filed December 13, 1995, and Ser. No. 60/008,606, filed December 14, 1995."

and replace with:

### --CROSS-REFERENCE TO RELATED APPLICATIONS

This application is a divisional of U.S. Application Serial No. 08/980,115, filed November 26, 1997 which claims benefit of U.S. Provisional Applications Serial No. 60/008,540, filed December 13, 1995; U.S. Provisional Application Serial No. 60/008,543, filed December 13, 1995; and U.S. Provisional Application Serial No. 60/008,606, filed December 14, 1995. Each of the foregoing Applications are hereby incorporated, in their entirety, by reference.

### ACKNOWLEDGMENTS

This invention was supported in part by grants from the National Institutes of Health grant number 1 R01 DK43787, and 5 R01 DK 41842. The U.S. Government may have rights in this invention.--

Please amend as follows:

Page 6, line 3, delete "**FIG. 3**" and insert --**FIGS. 3A-3R**--.

Page 6, line 31, delete "**FIG. 14**" and insert --**FIGS. 14A-14B**--.

At page 6, line 4, after "members of the nuclear receptor superfamily" insert -- SEQ ID NO: 1 rTR $\alpha$ ; SEQ ID NO: 2 hTR $\alpha$ ; SEQ ID NO: 3 hTR $\beta$ ; SEQ ID NO: 4 hRAR $\alpha$ ; SEQ ID NO: 5 hRAR $\gamma$ ; SEQ ID NO: 6 hRXR $\alpha$ ; SEQ ID NO: 7 hRXR $\beta$ ; SEQ ID NO: 8 hPPAR $\alpha$ ; SEQ ID NO: 9 hPPAR $\beta$ ; SEQ ID NO: 10 hPPAR $\gamma$ ; SEQ ID NO: 11 hVDR; SEQ ID NO: 12 hER; SEQ ID NO: 13 hGR; SEQ ID NO: 14 hPR; SEQ ID NO: 15 hMR; and SEQ ID NO: 16 hAR--.

Page 7, line 4, delete "**FIG. 17**" and insert --**FIGS. 17A-17B**--.

Page 23, line 14, delete "**FIG. 3**" and insert --**FIGS. 3A-3R**--.

Page 23, line 15, delete "FIG. 3" and insert --FIGS. 3A-3R--.

Page 23, line 17, delete "FIG. 3" and insert --FIGS. 3A-3R--.

Page 23, line 19, delete "FIG. 3" and insert --FIGS. 3A-3R--.

Page 23, line 28, delete "FIG. 3" and insert --FIGS. 3A-3R--.

Page 23, line 3, delete "FIG. 3" and insert --FIGS. 3A-3R--.

On page 60, line 4, after "in" delete "6".

Page 61, line 11, delete "FIG. 14" and insert --FIGS. 14A-14B--.

On page 70, line 29, after "in" delete "6".

Page 72, line 19, delete "FIG. 17" and insert --FIGS. 17A-17B--.

Page 75, line 21, delete "FIG. 3. FIG. 3" and insert --FIGS. 3A-3R. FIGS. 3A-3R--.

Page 75, line 23, delete "FIG. 3" and insert --FIGS. 3A-3R--.

Page 75, line 26, delete "FIG. 3" and insert --FIGS. 3A-3R--.

Please renumber pages 89-120 of the Claims to be pages 378-409.

Please renumber pages 121-409 of the Appendices to be pages 89-377.

#### IN THE DRAWINGS

In Figure 6, the bond in the attached red lined figure should be removed. A corrected Figure 6 is submitted and is also submitted as a formal drawing to the Official Draftsperson.

#### IN THE CLAIMS

Please cancel claims 1-17, 19-40, and 42-60.

Please amend claims 18 and 41 as follows:

18. (Amended) A peptide, peptidomimetic or synthetic [molecule] compound capable of selectively modulating the activity of a thyroid hormone receptor (TR) isoform, identified by the method [of any one of claims 8 or 17,] comprising:  
modeling test peptide, peptidomimetic or synthetic compounds that fit spatially and preferentially into a TR ligand binding domain (TR LBD) isoform of interest using

an atomic structural model of a TR LBD isoform bound to a test compound, wherein said atomic structural model is generated utilizing data from Appendix 3, 4, 5, 6, 7 or 8,  
screening said test compounds in a biological assay for TR isoform activity  
characterized by binding of a test compound to a TR LBD isoform, and  
identifying a test compound that selectively modulates the activity of a TR  
isoform, with the proviso that said [molecule] compound, is other than a thyronine or  
thyronine-like compound disclosed in a reference cited in Appendix I.

41. (Amended) A peptide, peptidomimetic or synthetic [molecule] compound  
that selectively modulates the activity of a thyroid hormone receptor (TR) compared to  
other nuclear hormone receptors, identified by the method [of any one of claims 19 or  
40,] comprising:

modeling compounds which fit spatially into a TR ligand binding domain (TR  
LBD) using an atomic structural model of a TR LBD, wherein said atomic structural  
model is generated utilizing data from Appendix 3, 4, 5, 6, 7 or 8,

selecting a compound comprising conformationally constrained structural features  
that interact with conformationally constrained residues of a TR LBD,

identifying in a biological assay for TR activity a compound that selectively binds  
to a TR LBD compared to other nuclear receptors, whereby a compound that selectively  
modulates a TR is identified, with the proviso that said [molecule] compound is other  
than a thyronine or thyronine-like compound disclosed in a reference cited in Appendix I.

Please insert the following claims:

--61. A peptide, peptidomimetic or synthetic compound wherein said compound  
is a thyroid hormone receptor (TR) agonist or antagonist ligand, identified by the method  
comprising the steps of:



providing the atomic coordinates of a TR ligand binding domain (TR LBD) to a computerized modeling system, wherein said atomic coordinates are generated utilizing data from Appendix 3, 4, 5, 6, 7 or 8;

modeling ligands which fit spatially into the TR LBD; and

identifying in a biological assay for TR activity a ligand which increases or decreases the activity of said TR, whereby a TR agonist or antagonist is identified, with the proviso that said compound is other than a thyronine or thyronine-like compound disclosed in a reference cited in Appendix I.

62. A peptide, peptidomimetic or synthetic compound wherein said compound is a thyroid hormone receptor (TR) agonist or antagonist ligand that selectively modulates the activity of a TR compared to other nuclear receptors, identified by the method comprising the steps of:

providing the atomic coordinates of a TR ligand binding domain (TR LBD) to a computerized modeling system, wherein said atomic coordinates are generated utilizing data from Appendix 3, 4, 5, 6, 7 or 8;

modeling ligands which fit spatially into the TR LBD and which interact with conformationally constrained residues of a TR LBD conserved among TR isoforms; and

identifying in a biological assay for TR activity a ligand which selectively binds to said TR and increases or decreases the activity of said TR, whereby a TR agonist or antagonist that selectively modulates the activity of a TR is identified, with the proviso that said molecule is other than a thyronine or thyronine-like compound disclosed in a reference cited in Appendix I.--

#### REMARKS

Page 1 of the Specification is amended to eliminate the duplicative "Cross-reference to Related Applications" and to correctly place the "Acknowledgements" section following the "Cross-reference to Related Applications." Further, the language of the "Cross-reference to Related Applications" has been modified to comport with the requirements of MPEP § 210.11 (version 7, July 1998, pg. 200-55).

The Specification is amended to properly refer to FIGS. 3A-3R, 14A-14B, and 17A-17B. Support for this amendment can be found at pages 6-8 of the specification as filed.

In the specification, the brief description of Figure 3 is amended to add the SEQ ID NO: identifier for each sequence presented in that figure. No new matter has been added by this Amendment.

The pages of the Specification are renumbered so that the Appendices are placed before the claims.

The additional bond in incorrect Figure 6 as noted above represents a typographical error in the structure of the molecule Dimit. The chemical structure of Dimit is correctly depicted in other portions of the present application. For example, the correct structure of Dimit is provided in the atomic coordinates of Appendix 3 as well as in Figure 22. Additionally, the correct structure of Dimit is provided in Figure 6 of the priority Provisional Application Serial No. 60/008,606 as filed on December 14, 1995. Accordingly, the correction of Figure 6 in the present application does not represent new matter or change the scope of the application as filed.

Claims 18 and 41 have been amended to include the language of the claims upon which these claims were dependent. The new language in claims 18 and 41 comes from allowed claims 8 and 19, respectively. Support for the new claims 61 and 62 can be found in the original versions of claims 18 and 41, and in the allowed claims 17 and 40.

None of the above amendments constitute new matter. The Applicant respectfully requests the Examiner to enter the above amendments prior to examination of the application.

If in the opinion of the Examiner, a telephone conference would expedite the prosecution of the subject application, the Examiner is invited to call the undersigned at (650) 843-5000.

The Commissioner is hereby authorized to charge any underpayment of the following fees associated with this communication, or credit any overpayment to Deposit Account No. 03-3117:

[X] Any national application filing fees under 37 CFR 1.16.

[illegible]

Respectfully submitted,  
COOLEY GODWARD LLP

Madison C. Jellins  
Reg. No. 35,555

1 NUCLEAR RECEPTOR LIGANDS AND LIGAND BINDING DOMAINS  
23 ACKNOWLEDGMENTS

4 This invention was supported in part by grants from the National Institutes of Health  
5 grant number 1 R01 DK 43787 and 5 R01 DK 41842. The U.S. Government may have  
6 certain rights in this invention.  
7

8 CROSS-REFERENCE TO RELATED APPLICATIONS

9 This application claims the benefit of the following provisional applications: United  
10 States Ser. No. 60/008,540 and 60/008,543, filed December 13, 1995, and Ser. No.  
11 60/008,606, filed December 14, 1995. This application claims the benefit of the following  
12 U.S. patent application: United States Ser. No. 08/764,870, filed December 13, 1996.  
13

14 INTRODUCTION15 Technical Field

16 This invention relates to computational methods for designing ligands that bind to  
17 nuclear receptors, crystals of nuclear receptors, synthetic ligands of nuclear receptors and  
18 methods of using synthetic ligands.  
19

20 Background

21 Nuclear receptors represent a superfamily of proteins that specifically bind a  
22 physiologically relevant small molecule, such as hormone or vitamin. As a result of a  
23 molecule binding to a nuclear receptor, the nuclear receptor changes the ability of a cell to  
24 transcribe DNA, i.e. nuclear receptors modulate the transcription of DNA, although they  
25 may have transcription independent actions. Unlike integral membrane receptors and  
26 membrane associated receptors, the nuclear receptors reside in either the cytoplasm or  
27 nucleus of eukaryotic cells. Thus, nuclear receptors comprise a class of intracellular, soluble  
28 ligand-regulated transcription factors.

1 Nuclear receptors include receptors for glucocorticoids (GRs), androgens (ARs),  
2 mineralocorticoids (MRs), progestins (PRs), estrogens (ERs), thyroid hormones (TRs),  
3 vitamin D (VDRs), retinoids (RARs and RXRs), peroxisomes (XPARs and PPARs) and  
4 icosanoids (IRs). The so called "orphan receptors" are also part of the nuclear receptor  
5 superfamily, as they are structurally homologous to the classic nuclear receptors, such as  
6 steroid and thyroid receptors. To date, ligands have not been identified with orphan  
7 receptors but it is likely that small molecule ligands will be discovered in the near future for  
8 this class of transcription factors. Generally, nuclear receptors specifically bind  
9 physiologically relevant small molecules with high affinity and apparent  $K_d$ 's are commonly  
10 in the 0.01 - 20 nM range, depending on the nuclear receptor/ligand pair.

11 Development of synthetic ligands that specifically bind to nuclear receptors has been  
12 largely guided by the trial and error method of drug design despite the importance of nuclear  
13 receptors in a myriad of physiological processes and medical conditions such as hypertension,  
14 inflammation, hormone dependent cancers (e.g. breast and prostate cancer), modulation of  
15 reproductive organ function, hyperthyroidism, hypercholesterolemia and obesity. Previously,  
16 new ligands specific for nuclear receptors were discovered in the absence of information on  
17 the three dimensional structure of a nuclear receptor with a bound ligand. Before the present  
18 invention, researchers were essentially discovering nuclear receptor ligands by probing in the  
19 dark and without the ability to visualize how the amino acids of a nuclear receptor held a  
20 ligand in its grasp.

21 Consequently, it would be advantageous to devise methods and compositions for  
22 reducing the time required to discover ligands to nuclear receptors, synthesize such  
23 compounds and administer such compounds to organisms to modulate physiological processes  
24 regulated by nuclear receptors.

25  
26

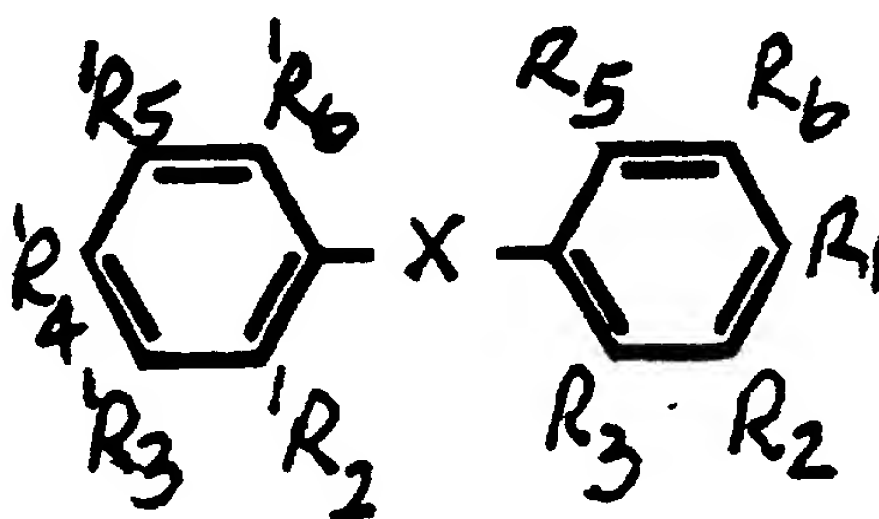


## SUMMARY OF THE INVENTION

The present invention provides for crystals of nuclear receptor ligand binding domains with a ligand bound to the ligand binding domain (LBD). The crystals of the present invention provide excellent atomic resolution of the amino acids that interact with nuclear receptor ligand, especially thyroid receptor ligands. The three dimensional model of a nuclear receptor LBD with a ligand bound reveals a previously unknown structure for nuclear receptors and shows that the ligand is bound in a water inaccessible binding cavity of the ligand binding domain of the nuclear receptor.

The present invention also provides for computational methods using three dimensional models of nuclear receptors that are based on crystals of nuclear receptor LBDs. Generally, the computational method of designing a nuclear receptor ligand determines which amino acid or amino acids of a nuclear receptor LBD interact with a chemical moiety (at least one) of the ligand using a three dimensional model of a crystallized protein comprising a nuclear receptor LBD with a bound ligand, and selecting a chemical modification (at least one) of the chemical moiety to produce a second chemical moiety with a structure that either decreases or increases an interaction between the interacting amino acid and the second chemical moiety compared to the interaction between the interacting amino acid and the corresponding chemical moiety on the natural hormone.

Also provided is a method of modulating the activity of a nuclear receptor. The method can be *in vitro* or *in vivo*. The method comprises administering *in vitro* or *in vivo* a sufficient amount of a compound of the following formula:



FORMULA I.

where the compound fits specially and preferentially into a nuclear hormone receptor LBD of interest. The method is exemplified by modulating the activity of a thyroid receptor (TR).

1 For modulating TR activity, a compound of Formula I is employed that fits spacially and  
2 preferentially into a TR ligand binding domain (TR LBD), including compounds specific for  
3 a TR LBD isoform of interest. Of particular interest are the TR LBD isoforms  $\alpha$  (TR- $\alpha$ ) and  
4  $\beta$  (TR- $\beta$ ). Additional compounds of interest include derivatives of Formula I, such as those  
5 compounds having the biphenyl ( $\phi$ -X- $\phi$ ) or single phenyl ( $\phi$ -X or X- $\phi$ ) nucleus of Formula I  
6 and its corresponding substituent groups described herein. Compounds that are iteratively  
7 designed using structural information gleaned from these compounds and which modulate  
8 nuclear hormone receptor activity also are of interest.

9 The present invention also includes a method for identifying a compound capable of  
10 selectively modulating the activity of a nuclear receptor. This aspect of the invention is  
11 exemplified by a method for identifying a compound capable of selectively modulating the  
12 activity of a TR isoform. The method comprises modeling test compounds that fit spacially  
13 and preferentially into a TR LBD isoform of interest using an atomic structural model of a  
14 TR LBD isoform bound to a test compound, screening the test compounds in a biological  
15 assay for TR isoform activity characterized by binding of a test compound to a TR LBD  
16 isoform, and identifying a test compound that selectively modulates the activity of a TR  
17 isoform. The compounds may be those of Formula I or derivatives thereof, including  
18 compounds having a biphenyl or single phenyl nucleus of Formula I.

19 Further included is a method for identifying agonist or antagonist ligands of a nuclear  
20 receptor using the atomic coordinates of a LBD in conjunction with a computerized modeling  
21 system. This aspect of the invention is exemplified by identifying a TR agonist or antagonist  
22 ligand by providing the atomic coordinates of a TR LBD to a computerized modeling system,  
23 modeling ligands which fit spacially into the TR LBD, and identifying in a biological assay  
24 for TR activity a ligand which increases or decreases TR activity. The compounds can be  
25 those of Formula I or derivatives thereof, including compounds having a biphenyl or single  
26 phenyl nucleus of Formula I.

27 Also provided is a method of identifying a compound that selectively modulates the  
28 activity of one type of nuclear receptor compared to other nuclear hormone receptors. The  
29 method is exemplified by modeling test compounds which fit spacially into a TR LBD using  
30 an atomic structural model of a TR LBD, selecting a compound comprising conformationally  
31 constrained structural features that interact with conformationally constrained residues of a

1 TR LBD, and identifying in a biological assay for TR activity a compound that selectively  
2 binds to a TR LBD compared to other nuclear receptors. The conformationally constrained  
3 features involved in receptor-selective ligand binding can be identified by comparing atomic  
4 models of receptor isoforms bound to the same and/or different ligands. The methods  
5 facilitate design and selection of compounds that have increased selectivity for a particular  
6 nuclear receptor. The compounds may be those of Formula I or derivatives thereof,  
7 including compounds having the biphenyl or single phenyl nucleus of Formula I.

8 Another aspect of the invention is a method for increasing the receptor selectivity of a  
9 compound for a particular type of nuclear receptor. This involves the chemical modification  
10 of a substituent group of a compound of Formula I to generate compounds which have  
11 increased selectivity for one type of receptor. For example, chemical modification of a  
12 substituent group of the compound of Formula I can be used to introduce additional  
13 constraints into a compound that modulates TR activity to increase its selectivity *in vivo* for  
14 TR-type receptors. Additional constraints also may be added for stability. The modified  
15 groups will preferably interact with a conformationally constrained structural feature of a TR  
16 LBD that is conserved among TR isoforms. A more preferred method comprises selecting  
17 compounds having conformationally constrained groups that interact with conformationally  
18 constrained residues of a TR LBD conserved among TR isoforms. The compounds can be  
19 those of Formula I or derivatives thereof, including compounds having the biphenyl or single  
20 phenyl nucleus of Formula I.

21 The invention finds use in the selection and characterization of peptide,  
22 peptidomimetic or synthetic compounds identified by the methods of the invention,  
23 particularly new lead compounds useful in treating disorders related to nuclear receptor-based  
24 deficiencies, including TR-related disorders. For TR-related disorders, the compounds and  
25 methods of the invention can be used to modulate TR activity by administering to a mammal  
26 in need thereof a sufficient amount of compound of Formula I or derivative thereof that fits  
27 spacially and preferentially into a TR LBD.

## 28 29 BRIEF DESCRIPTION OF THE DRAWINGS

30 FIG. 1 is a diagram illustrating computational methods for designing ligands that  
31 interact with nuclear receptors of the nuclear receptor superfamily.

1        **FIG. 2** is a schematic representation of nuclear receptor structures, indicating regions  
2 of homology within family members and functions of the various domains.

3        **FIG. 3** shows the aligned amino acid sequences of the ligand binding domains of  
4 several members of the nuclear receptor superfamily.

5        **FIG. 4** is a ribbon drawing of the rat TR- $\alpha$  LBD with secondary structure elements  
6 labelled. The ligand (magenta) is depicted as a space-filling model. Alpha helices and coil  
7 conformations are yellow, beta strands are blue.

8        **FIG. 5** shows two cross-sections of a space-filling model of rat TR- $\alpha$  exposing the  
9 ligand (magenta) tightly packed within the receptor.

10       **FIG. 6** is a schematic of the ligand binding cavity. Residues which interact with the  
11 ligand appear approximately at the site of interaction. Hydrogen bonds are shown as dashed  
12 lines between the bonding partners; distances for each bond are listed. Non-bonded contacts  
13 are shown as radial spokes which face toward interacting atoms.

14       **FIG. 7** is the distribution of crystallographic temperature factors in the refined rat  
15 TR- $\alpha$  LBD. The distribution is represented as a color gradation ranging from less than 15  
16 (dark blue) to greater than 35 (yellow-green).

17       **FIG. 8** is a ribbon drawing of the rat TR- $\alpha$  LBD showing the c-terminal activation  
18 domain to ligand. Residues which comprise the c-terminal activation domain (Pro393-  
19 Phe405) are depicted as a stick representation. Hydrophobic residues, particularly Phe401  
20 and Phe405 (blue) face inwards toward the ligand. Glu403 (red) projects outward into the  
21 solvent.

22       **FIG. 9** is an electrostatic potential surface of the rat TR- $\alpha$  LBD, calculated using  
23 GRAPH. Negative electrostatic potential is red; positive electrostatic potential is blue. The  
24 c-terminal activation domain forms a largely hydrophobic (white). The Glu403 is presented  
25 as a singular patch of negative charge (red).

26       **FIG. 10** is a diagram comparing agonists and antagonists for several nuclear  
27 receptors.

28       **FIG. 11** is the synthetic scheme for preparation of TS1, TS2, TS3, TS4 and TS5.

29       **FIG. 12** is the synthetic scheme for preparation of TS6 and TS7.

30       **FIG. 13** is the synthetic scheme for preparation of TS8.

31       **FIG. 14** is the synthetic scheme for preparation of TS10.

1        **FIG. 15** depicts the chemical structures of several TR ligands.

2        **FIG. 16** is a graph illustrating competition assays in which T<sub>3</sub> and Triac compete with  
3 labeled T<sub>3</sub> for binding to human TR- $\alpha$  or human TR- $\beta$ .

4        **FIG. 17** depicts a Scatchard analysis of labelled T<sub>3</sub> binding to TR- $\alpha$  and TR- $\beta$ .

5        **FIG. 18** is a chart showing the effect of TS-10 on the transcriptional regulation of the  
6 DR4-ALP reporter gene in the presence or absence of T<sub>3</sub> as assayed in TRAF $\alpha$ 1 reporter  
7 cells.

8        **FIG. 19** is a chart showing the effect of TS-10 on the transcriptional regulation of the  
9 DR4-ALP reporter gene in the presence or absence of T<sub>3</sub> as assayed in TRAF $\beta$ 1 reporter  
10 cells.

11        **FIG. 20** is a chart showing the effect of TS-10 on the transcriptional regulation of the  
12 DR4-ALP reporter gene in the presence or absence of T<sub>3</sub> as assayed in HepG2, a liver  
13 reporter cell line.

14        **FIG. 21** is a partial ribbon drawing of TR- $\alpha$  LBD with T<sub>3</sub> in the ligand binding  
15 cavity. Selected interacting amino acids are labelled, including Ile221, Ile222 and Ser260,  
16 Ala263, Ile299 and Leu 276.

17        **FIG. 22** is a partial ribbon drawing of TR- $\alpha$  LBD with T<sub>3</sub> and Dimit superimposed in  
18 the ligand binding cavity. Interactions with Ile221, Ile222, Ala260, Ile 299 and Leu276 are  
19 labelled.

20        **FIG. 23** is a partial ribbon drawing of TR- $\alpha$  LBD with T<sub>3</sub>, illustrating the three  
21 Arginine residues (Arg228, Arg262 and Arg 266 (dark stick figures)) of the polar pocket,  
22 three water molecules HOH502, HOH503 and HOH504, with hydrogen bonds indicated by  
23 dotted lines.

24        **FIG. 24** is a partial ribbon drawing of TR- $\alpha$  LBD with Triac, illustrating the three  
25 Arginine residues (dark stick figures) of the polar pocket, water molecules (HOH503,  
26 HOH504 and HOH600), with hydrogen bonds indicated by dotted lines.

27        **FIG. 25** is a partial ribbon drawing of the TR- $\alpha$  LBD with T<sub>3</sub> and Triac  
28 superimposed in the ligand binding cavity. The drawing shows several interacting amino  
29 acid residues in the polar pocket that remain unchanged whether T<sub>3</sub> or Triac occupies the  
30 ligand binding cavity: Arg262, Asn179, HOH503 and HOH504, and Ser277. Both Arg228  
31 and Arg 266 occupy two different positions, depending on whether T<sub>3</sub> or Triac is bound.



1        **FIG. 26A and 26B** are stereochemical representations of the TR- $\alpha$  LBD with Dimit  
2 bound.

3        **FIG. 27** is a partial ribbon drawing of TR- $\beta$  LBD with GC-1 in the ligand binding  
4 cavity. Amino acids Arg282, Arg316, Arg320, Asn 331 and His435 are labelled.

5        **FIG. 28** is a partial ribbon drawing of TR- $\beta$  LBD with Triac in the ligand binding  
6 cavity. Amino acids Arg282, Arg316, Arg320, Asn331 and His435 are labelled.

7        **FIG. 29** is a partial ribbon drawing of TR- $\beta$ LBD with GC-1 (Blue) overlayed with  
8 TR- $\alpha$  LBD with Dimit (Red) in the ligand binding cavities. Amino acids Arg228, Arg262,  
9 Arg266 and Ser277 (TR- $\alpha$  LBD), and Arg282, Arg316, Arg320 and Asn331 (TR- $\beta$  LBD)  
10 are labelled.

11        **FIG. 30** is a partial ribbon drawing of TR- $\beta$  LBD with Triac (Blue) overlayed with  
12 TR- $\alpha$  LBD with Triac (Red) in the ligand binding cavities. Amino acids Arg228, Arg262,  
13 Arg266, Ser277 and His381 (TR- $\alpha$  LBD), and Arg282, Arg316, Arg320 and His435 (TR- $\beta$   
14 LBD) are labelled.

15        **FIG. 31** is a graph showing competition curves comparing wildtype TR- $\alpha$  and TR- $\beta$   
16 to a variant TR- $\beta$  having a single amino acid substitution in the ligand binding domain.

17        **FIG. 32** shows atomic numbering for thyronine-like ligands.

18        **APPENDIX 1** is an appendix of references.

19        **APPENDIX 2** is a chart of amino acids that interact with a TR ligand, for TR  
20 complexed with Dimit, Triac, IpBr<sub>2</sub>, T<sub>3</sub> and GC-1.

21        **APPENDIX 3** is a chart of atomic coordinates for the crystal of rat TR- $\alpha$  LBD  
22 complexed with Dimit.

23        **APPENDIX 4** is a chart of atomic coordinates for the crystal of rat TR- $\alpha$  LBD  
24 complexed with Triac.

25        **APPENDIX 5** is a chart of atomic coordinates for the crystal of rat TR- $\alpha$  LBD  
26 complexed with IpBr<sub>2</sub>.

27        **APPENDIX 6** is a chart of atomic coordinates for the crystal of rat TR- $\alpha$  LBD  
28 complexed with T<sub>3</sub>.

29        **APPENDIX 7** is a chart of atomic coordinates for the crystal of human TR- $\beta$  LBD  
30 complexed with Triac.

1           **APPENDIX 8** is a chart of atomic coordinates for the crystal of human TR- $\beta$ -LBD  
2 complexed with GC-1.

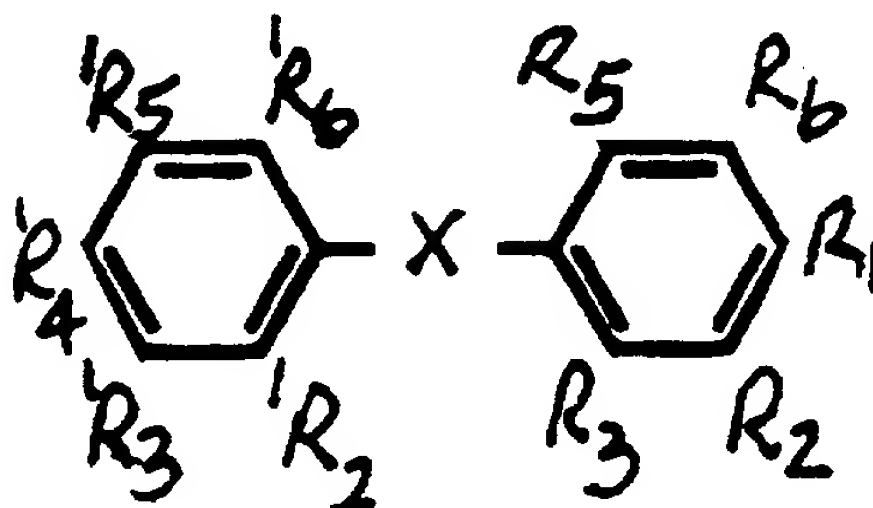
4                           DETAILED DESCRIPTION OF THE INVENTION

5       **INTRODUCTION**

6           The present invention provides new methods, particularly computational methods, and  
7 compositions for the generation of nuclear receptor synthetic ligands based on the three  
8 dimensional structure of nuclear receptors, particularly the thyroid receptor (herein referred  
9 to as "TR"). Previously, the lack of three dimensional structural information about the  
10 ligand binding domain of a nuclear receptor thwarted the field of nuclear receptor drug  
11 discovery, especially the absence of three dimensional structural information relating to a  
12 nuclear receptor with a ligand bound.

13           Described herein for the first time are crystals and three dimensional structural  
14 information from a nuclear receptor's ligand binding domain (LBD) with a ligand bound.  
15 The structure of the TR LBD complexed with 3,5,3'-triiodothyronine (T<sub>3</sub>), 3,5-dibromo-3'-  
16 isopropylthyronine (IpBr<sub>2</sub>), 3,5- dimethyl-3'-isopropylthyronine (Dimit), and 3,5,3'-  
17 triiodothyroacetic acid (Triac), 3,5-dimethyl-4-(4'-hydroxy-3'isopropylbenzyl)-phenoxy acetic  
18 acid (GC1) are exemplified. Such crystals offer superior resolution at the atomic level and  
19 the ability to visualize the coordination of nuclear receptor ligands by amino acids that  
20 comprise the LBD. The present invention also provides computational methods for designing  
21 nuclear receptor synthetic ligands using such crystal and three dimensional structural  
22 information to generate synthetic ligands that modulate the conformational changes of a  
23 nuclear receptor's LBD. Such synthetic ligands can be designed using the computational  
24 methods described herein and shown, in part, in **FIG. 1**. These computational methods are  
25 particularly useful in designing an antagonist or partial agonist to a nuclear receptor, wherein  
26 the antagonist or partial agonist has an extended moiety that prevents any one of a number of  
27 ligand-induced molecular events that alter the receptor's influence on the regulation of gene  
28 expression, such as preventing the normal coordination of the activation domain observed for  
29 a naturally occurring ligand or other ligands that mimic the naturally occurring ligand, such  
30 as an agonist. As described herein, synthetic ligands of nuclear receptors will be useful in  
31 modulating nuclear receptor activity in a variety of medical conditions.

Of particular interest is use of such ligands in a method of modulating TR activity in a mammal by administering to a mammal in need thereof a sufficient amount of a compound of Formula I,



where the compound fits spatially and preferentially into a TR LBD. By "fits spatially" is intended that the three-dimensional structure of a compound is accommodated geometrically by a cavity or pocket of a TR LBD. By "TR LBD" is intended a structural segment or segments of thyroid hormone receptor polypeptide chain folded in such a way so as to give the proper geometry and amino acid residue configuration for ligand binding. This is the physical arrangement of protein atoms in three-dimensional space forming a ligand binding pocket or cavity. By "fits spatially and preferentially" is intended that a compound possesses a three-dimensional structure and conformation for selectively interacting with a TR LBD. Compounds of interest also include derivatives of Formula I. By "derivatives of Formula I" is intended compounds that comprise at least a single phenyl scaffold ( $\phi$ -X or X- $\phi$ ) of the biphenyl scaffold ( $\phi$ -X- $\phi$ ) of Formula I which comprise the corresponding substituents of Formula I described herein. Compounds that are iteratively designed using structural information gleaned from these compounds and which modulate nuclear hormone receptor activity also are of interest. Preferred compounds of Formula I and its derivatives that fit spatially and preferentially into a TR LBD comprise the following substituents:

(i) an R1-substituent comprising an anionic group that interacts with a side chain nitrogen atom of an arginine corresponding to a residue from the group Arg228, Arg262, and Arg266 of human TR- $\alpha$ , and Arg282, Arg316 and Arg320 of human TR- $\beta$ , where the anionic group is about 1.7-4.0Å from the nitrogen atom;

- 1 (ii) an R2-substituent comprising a hydrophobic or hydrophilic group that fits  
2 spacially into the TR LBD;
- 3 (iii) an R3-substituent comprising a hydrophobic or hydrophilic group that  
4 interacts with a side chain atom of a serine, alanine and/or isoleucine corresponding to a  
5 residue from the group Ser260, Ala263 and Ile299 of human TR- $\alpha$ , and Ser314, Ala317 and  
6 Ile352 of human TR- $\beta$ , where the hydrophobic or hydrophilic group is about 1.7-4.0Å from  
7 the side chain atom;
- 8 (iv) an R5-substituent comprising a hydrophobic or hydrophilic group that interacts  
9 with a side chain atom of a phenylalanine and/or isoleucine corresponding to a residue from  
10 the group Phe218, Ile221 and Ile222 of human TR- $\alpha$ , and Phe272, Ile275 and Ile276 of  
11 human TR- $\beta$ , where the hydrophobic or hydrophilic group is about 1.7-4.0Å from the side  
12 chain atom;
- 13 (v) an R6-substituent comprising a hydrophobic or hydrophilic group that fits  
14 spacially into the TR LBD;
- 15 (vi) an X-substituent comprising a hydrophobic or hydrophilic group that interacts  
16 with a side chain atom of a leucine corresponding to a residue from the group Leu276 and  
17 Leu292 of human TR- $\alpha$ , and Leu 330 and Leu346 of human TR- $\beta$ , where the hydrophobic  
18 or hydrophilic group is about 1.7-4.0Å from the side chain atom;
- 19 (vii) an R2'-substituent comprising a hydrophobic or hydrophilic group that fits  
20 spacially into the TR LBD;
- 21 (viii) an R3'-substituent comprising a hydrophobic group that interacts with a side  
22 chain atom of a phenylalanine, glycine and/or methionine corresponding to a residue from  
23 the group Phe215, Gly290, and Met388 of human TR- $\alpha$ , and Phe269, Gly344, Met442 of  
24 human TR- $\beta$ , where the hydrophobic group is about 1.7-4.0Å from the side chain atom;
- 25 (ix) an R4'-substituent comprising an hydrogen bond donor or acceptor group that  
26 interacts with a side chain carbon or nitrogen atom of a histidine corresponding to residue  
27 His381 of human TR- $\alpha$ , and His435 of human TR- $\beta$ , where the hydrogen bond donor or  
28 acceptor group is about 1.7-4.0Å from the side chain atom;
- 29 (x) an R5'-substituent comprising a hydrophobic or hydrophilic group that fits  
30 spacially into the TR LBD;

(xi) and R6'-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD; and

where the compound is other than thyronine (T3), triiodothyronine (T4) or other thyronine-like compounds previously known and used in a TR treatment method, such as those referenced in Appendix I.

Examples of such substituents include the following:

where R<sub>1</sub> is

-O-CH<sub>2</sub>CO<sub>2</sub>H, -NHCH<sub>2</sub>CO<sub>2</sub>H, -CO<sub>2</sub>H, -CH<sub>2</sub>CO<sub>2</sub>H, -CH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H, -CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H, -CH<sub>2</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H, -CH<sub>2</sub>CH[NHCOCH<sub>2</sub>]<sub>2</sub>CO<sub>2</sub>H, -CH<sub>2</sub>CH[NHCO(CH<sub>2</sub>)<sub>15</sub>CH<sub>3</sub>]CO<sub>2</sub>H, -CH<sub>2</sub>CH[NH-FMOC]CO<sub>2</sub>H, -CH<sub>2</sub>CH[NH-tBOC]CO<sub>2</sub>H, or a carboxylate connected to the ring with a 0 to 3 carbon linker,  
-PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>CH<sub>2</sub>PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>CHNH<sub>2</sub>PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>CH[NHCOCH<sub>2</sub>]<sub>2</sub>PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>CH[NHCO(CH<sub>2</sub>)<sub>15</sub>CH<sub>3</sub>]PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>CH[NH-FMOC]PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>CH[NH-tBOC]PO<sub>3</sub>H<sub>2</sub>, or a phosphate or phosphonate connected to the ring with a 0 to 3 carbon linker,  
-SO<sub>3</sub>H, -CH<sub>2</sub>SO<sub>3</sub>H, -CH<sub>2</sub>CH<sub>2</sub>SO<sub>3</sub>H, -CH<sub>2</sub>CHNH<sub>2</sub>SO<sub>3</sub>H, -CH<sub>2</sub>CH[NHCOCH<sub>2</sub>]<sub>2</sub>SO<sub>3</sub>H, -CH<sub>2</sub>CH[NHCO(CH<sub>2</sub>)<sub>15</sub>CH<sub>3</sub>]SO<sub>3</sub>H, -CH<sub>2</sub>CH[NH-FMOC]SO<sub>3</sub>H, -CH<sub>2</sub>CH[NH-tBOC]SO<sub>3</sub>H, or a sulfate or sulfite connected to the ring with a 0 to 3 carbon linker, or acts as the functional equivalent of CH<sub>2</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H of T3 in the molecular recognition domain when bound to a TR, wherein R<sub>1</sub> can be optionally substituted with an amine,

where R<sub>2</sub> is

H, halogen, CF<sub>3</sub>, OH, NH<sub>2</sub>, SH, CH<sub>3</sub>, -Et, or acts as the functional equivalent of H in the molecular recognition domain when bound to a TR,

where R<sub>3</sub> is

-H, halogen, -CF<sub>3</sub>, -OH, -NH<sub>2</sub>, -N<sub>3</sub>, -SH, -CH<sub>3</sub>, -Et, or acts as the functional equivalent of I in the molecular recognition domain when bound to a TR,

where R<sub>5</sub> is



1        -H, halogen, -CF<sub>3</sub>, -OH, -NH<sub>2</sub>, -N<sub>3</sub>, -SH, -CH<sub>3</sub>, -Et, or acts as the functional  
 2        equivalent of I in the molecular recognition domain when bound to a TR, and R<sub>3</sub> can  
 3        be identical to R<sub>5</sub>,  
 4        where R<sub>6</sub> is  
 5        -H, halogen, -CF<sub>3</sub>, -OH, -NH<sub>2</sub>, -SH, -CH<sub>3</sub>, or acts as the functional equivalent of H  
 6        in the molecular recognition domain when bound to a TR, and R<sub>2</sub> can be identical to  
 7        R<sub>6</sub>,  
 8        where R<sub>2</sub>' is  
 9        -H, halogen, -CF<sub>3</sub>, -OH, -NH<sub>2</sub>, -N<sub>3</sub>, -SH, -CH<sub>3</sub>, -Et, or acts as the functional  
 10       equivalent of H in the molecular recognition domain when bound to a TR,  
 11       where R<sub>3</sub>' is any hydrophobic group, including  
 12       halogen, -CF<sub>3</sub>, -SH, alkyl, aryl, 5- or 6-membered heterocycle, cyano, or acts as the  
 13       functional equivalent of I in the molecular recognition domain when bound to a TR,  
 14       where R<sub>4</sub>' is  
 15       -H, halogen, -CF<sub>3</sub>, -OH, -NH<sub>2</sub>, NH<sub>3</sub>, -N(CH<sub>3</sub>)<sub>3</sub>, carboxylate, phosphonate, phosphate  
 16       or sulfate, -SH, -CH<sub>3</sub>, -Et, or alkyl, aryl or 5- or 6-membered heterocyclic aromatic  
 17       attached through urea or carbamate linkages to O or N or S at the R<sub>4</sub>' position, or  
 18       acts as the functional equivalent of OH in the molecular recognition domain when  
 19       bound to a TR,  
 20       where R<sub>5</sub>' is  
 21       -H, -OH, -NH<sub>2</sub>, -N(CH<sub>3</sub>)<sub>2</sub>, -SH, -NH<sub>3</sub>, -N(CH<sub>3</sub>)<sub>3</sub>, carboxylate, phosphonate, phosphate,  
 22       sulfate, branched or straight chain alkyl having 1 to 9 carbons, substituted or  
 23       unsubstituted aryl, wherein said substituted aryl is substituted with halogen or 1 to 5  
 24       carbon alkyl and wherein said aryl is optionally connected to the ring by a -CH<sub>2</sub>-,  
 25       aromatic heterocycle having 5 to 6 atoms, wherein said heterocycle may be substituted  
 26       with one or more groups selected from -OH, -NH<sub>2</sub>, -SH, -NH<sub>3</sub>, -N(CH<sub>3</sub>)<sub>3</sub>,  
 27       carboxylate, phosphonate, phosphate or sulfate, heteroalkyl, arylalkyl, heteroaryl  
 28       alkyl, polyaromatic, or polyheteroaromatic, wherein said R<sub>5</sub>' may be substituted with  
 29       polar or charged groups,  
 30       where R<sub>6</sub>' is

1 -H, halogen, -CF<sub>3</sub>, -OH, -NH<sub>2</sub>, -SH, -CH<sub>3</sub>, -Et, or acts as the functional equivalent of  
2 H in the molecular recognition domain when bound to a TR,

3 where X is

4 O, S, SO<sub>2</sub>, NH, NR<sub>7</sub>, CH<sub>2</sub>, CHR<sub>7</sub>, CR<sub>7</sub>R<sub>7</sub>, wherein R<sub>7</sub> is alkyl, aryl or 5- or  
5 6-membered heterocyclic aromatic,

6 and where the TR LBD ligand has an apparent K<sub>d</sub> for binding TR LBD of 1 μM or less.

7 Of particular interest are the class of compounds according to Formula I having the  
8 following substituents: where R<sub>1</sub> is carboxylate, phosphonate, phosphate or sulfite and is  
9 connected to the ring with a 0 to 3 carbon linker, R<sub>2</sub> is H, R<sub>3</sub> is -I, -Br, or -CH<sub>3</sub>, R<sub>5</sub> is -I, -  
10 Br, or -CH<sub>3</sub>, R<sub>6</sub> is H, R<sub>2</sub>' is H, R<sub>3</sub>' is -I, -Br, -CH<sub>3</sub>, -iPr, -phenyl, benzyl, or 5- or 6-  
11 membered ring heterocycles, R<sub>4</sub>' is -OH, -NH<sub>2</sub>, and -SH, R<sub>5</sub>' is -H, -OH, -NH<sub>2</sub>, -N(CH<sub>3</sub>)<sub>2</sub> -  
12 SH -NH<sub>3</sub>, -N(CH<sub>3</sub>)<sub>3</sub>, carboxylate, phosphonate, phosphate, sulfate, branched or straight chain  
13 alkyl having 1 to 9 carbons, substituted or unsubstituted aryl, wherein said substituted aryl is  
14 substituted with halogen or 1 to 5 carbon alkyl and wherein said aryl is optionally connected  
15 to the ring by a -CH<sub>2</sub>-, aromatic heterocycle having 5 to 6 atoms, wherein said heterocycle  
16 may be substituted with one or more groups selected from -OH, -NH<sub>2</sub>, -SH, -NH<sub>3</sub>, -N(CH<sub>3</sub>)<sub>3</sub>,  
17 carboxylate, phosphonate, phosphate or sulfate, heteroalkyl, arylalkyl, heteroaryl alkyl,  
18 polyaromatic, or polyheteroaromatic, wherein said R<sub>5</sub>' may be substituted with polar or  
19 charged groups, and R<sub>6</sub>' is H.

20 The present invention also includes a method for identifying a compound capable of  
21 selectively modulating the activity of a TR isoform. By "modulating" is intended increasing  
22 or decreasing activity of a TR. By "TR isoform" is intended TR proteins encoded by  
23 subtype and variant TR genes. This includes TR-α and TR-β isoforms encoded by different  
24 genes (e.g., *thra* and *thrb*) and variants of the same genes (e.g., *thrb1* and *thrb2*). The  
25 method comprises the steps of modeling test compounds that fit spacially and preferentially  
26 into a TR LBD isoform of interest using an atomic structural model of a TR LBD isoform  
27 bound to a test compound, screening the test compounds in a biological assay for TR isoform  
28 activity characterized by binding of a test compound to a TR LBD isoform, and identifying a  
29 test compound that selectively modulates the activity of a TR isoform. By "modeling" is  
30 intended quantitative and qualitative analysis of receptor-ligand structure/function based on  
31 three-dimensional structural information and receptor-ligand interaction models. This

1 includes conventional numeric-based molecular dynamic and energy minimization models,  
2 interactive computer graphic models, modified molecular mechanics models, distance  
3 geometry and other structure-based constraint models. Modeling is preferably performed  
4 using a computer and may be further optimized using known methods.

5 For selectively modulating activity of a TR isoform, such as TR- $\alpha$  or TR- $\beta$ , a  
6 sufficient amount of a compound that fits spatially and preferentially into TR LBD isoform is  
7 provided *in vitro* or *in vivo* to achieve the desired end result. TR- $\alpha$  isoform selectivity can  
8 be accomplished with a compound comprising an anionic group that interacts with an oxygen  
9 or carbon of a serine residue corresponding to Ser277 of human TR- $\alpha$ , where the anionic  
10 group is about 1.7-4.0Å from the side chain atom. TR- $\beta$  isoform selectivity can be  
11 accomplished with a compound comprising an anionic group that interacts with the side chain  
12 nitrogen of an asparagine corresponding to Asn331 of human TR- $\beta$ , where the anionic group  
13 is about 1.7-4.0Å from the side chain nitrogen atom.

14 The present invention further includes a method for identifying a TR agonist or  
15 antagonist ligand by providing the atomic coordinates of a TR LBD to a computerized  
16 modeling system, modeling ligands which fit spacially into the TR LBD, and identifying in a  
17 biological assay for TR activity a ligand which increases or decreases the activity of the TR.

18 The invention also involves a method for increasing receptor selectivity of a  
19 compound of Formula I or derivatives thereof for a TR-type receptor versus other nuclear  
20 receptors by selecting a compound that interacts with conformationally constrained residues  
21 of a TR LBD that are conserved among TR isoforms. "Conformationally constrained" is  
22 intended to refer to the three-dimensional structure of a chemical or moiety thereof having  
23 certain rotations about its bonds fixed by various local geometric and physical-chemical  
24 constraints. In designing and selecting compounds having increased specificity for TRs  
25 compared to other nuclear receptors, the following methods of the invention can be used.  
26 One method involves comparing atomic models of a first TR LBD isoform bound to a  
27 compound with a second TR LBD isoform bound to the same compound, identifying atoms  
28 of the TR LBD and compounds which interact, and designing or selecting a compound that  
29 interacts with TR LBD residues comprising a conformationally constrained structural feature  
30 that is conserved between the TR LBD isoforms. Another method relates to comparing a  
31 first TR LBD complexed with a first compound to a second TR LBD complexed with a

1 second compound having one or more different substituents compared to the first compound,  
2 identifying atoms of the TR LBD and compounds which interact, and designing or selecting  
3 compounds that interact with TR LBD residues comprising a conformationally constrained  
4 structural feature that is conserved between the TR LBD isoforms. The methods also  
5 facilitate identification of structural and conformationally constrained interactions that are  
6 conserved between compounds that bind to a TR LBD. The methods are exemplified by  
7 comparing atomic models of a first TR LBD isoform complexed with a first compound of  
8 Formula I to a second TR LBD isoform complexed with the first compound, or a second  
9 compound of Formula I having different substituents than the first compound. For example,  
10 a TR- $\alpha$  LBD bound to a natural hormone such as T3 is compared to a TR- $\beta$  LBD bound to  
11 an organic thyronine-like compound such as GC-1. Conserved contacts are identified which  
12 are made between atoms of the different compounds and atoms of the TR LBDs, and the  
13 fiducial and adjustable components identified. Compounds selective for TR are identified in  
14 a biological assay for TR activity that assays for selective binding to a TR and/or TR LBD  
15 compared to other nuclear receptors. Conventional assays for TR and other nuclear  
16 receptors may be conducted in parallel or serially, including those assays described herein.  
17 Automatable methods are preferred. The methods facilitate design and selection of  
18 compounds comprising cyclic carbon and substituent atoms that interact with a constrained  
19 side chain and/or main chain atom of a TR LBD residue.

20 In another aspect of the invention, the methods described herein are useful for  
21 selecting peptides, peptidomimetics or synthetic molecules that modulate TR activity.  
22 Methods of the invention also find use in characterizing structure/function relationships of  
23 natural and synthetic TR-ligands. Molecules of particular interest are new thyronine-like  
24 compounds other than T3, T4 and other thyronine-like compounds previously known and  
25 used for treating TR-related disorders. New compounds of the invention include those which  
26 bind to a TR LBD isoform with greater affinity than T3 or T4 and those which exhibit  
27 isoform-specific binding affinity.

## 28 29 **APPLICABILITY TO NUCLEAR RECEPTORS**

30 The present invention, particularly the computational methods, can be used to design  
31 drugs for a variety of nuclear receptors, such as receptors for glucocorticoids (GRs),

1 androgens (ARs), mineralocorticoids (MRs), progestins (PRs), estrogens (ERs), thyroid  
2 hormones (TRs), vitamin D (VDRs), retinoid (RARs and RXRs), icosanoid (IRs), and  
3 peroxisomes (XPARS and peroxisomal proliferators (PPAP)). The present invention can also  
4 be applied to the "orphan receptors," as they are structurally homologous in terms of  
5 modular domains and primary structure to classic nuclear receptors, such as steroid and  
6 thyroid receptors. The amino acid homologies of orphan receptors with other nuclear  
7 receptors ranges from very low (<15%) to in the range of 35% when compared to rat  
8 RAR $\alpha$  and human TR- $\beta$  receptors, for example. In addition, as is revealed by the X-ray  
9 crystallographic structure of the TR and structural analysis disclosed herein, the overall  
10 folding of liganded superfamily members is likely to be similar. Although ligands have not  
11 been identified with orphan receptors, once such ligands are identified one skilled in the art  
12 will be able to apply the present invention to the design and use of such ligands, as their  
13 overall structural modular motif will be similar to other nuclear receptors described herein.

#### 14 15 *Modular Functional Domains Of Nuclear receptors*

16 The present invention will usually be applicable to all nuclear receptors, as discussed  
17 herein, in part, to the patterns of nuclear receptor activation, structure and modulation that  
18 have emerged as a consequence of determining the three dimensional structures of nuclear  
19 receptors with different ligands bound, notably the three dimensional structures or  
20 crystallized protein structure of the ligand binding domains for TR- $\alpha$  and TR- $\beta$ . Proteins of  
21 the nuclear receptor superfamily display substantial regions of amino acid homology, as  
22 described herein and known in the art see FIG. 2. Members of this family display an  
23 overall structural motif of three modular domains (which is similar to the TR three modular  
24 domain motif):

- 25 1) a variable amino-terminal domain;
- 26 2) a highly conserved DNA-binding domain (DBD); and
- 27 3) a less conserved carboxyl-terminal LBD.

28 The modularity of this superfamily permits different domains of each protein to separately  
29 accomplish different functions, although the domains can influence each other. The separate  
30 function of a domain is usually preserved when a particular domain is isolated from the  
31 remainder of the protein. Using conventional protein chemistry techniques a modular domain



1 can sometimes be separated from the parent protein. Using conventional molecular biology  
2 techniques each domain can usually be separately expressed with its original function intact  
3 or chimerics of two different nuclear receptors can be constructed, wherein the chimerics  
4 retain the properties of the individual functional domains of the respective nuclear receptors  
5 from which the chimerics were generated.

6 **FIG. 2** provides a schematic representation of family member structures, indicating  
7 regions of homology within family members and functions of the various domains.

### 8 9 *Amino Terminal Domain*

10 The amino terminal domain is the least conserved of the three domains and varies  
11 markedly in size among nuclear receptor superfamily members. For example, this domain  
12 contains 24 amino acids in the VDR and 603 amino acids in the MR. This domain is  
13 involved in transcriptional activation and in some cases its uniqueness may dictate selective  
14 receptor-DNA binding and activation of target genes by specific receptor isoforms. This  
15 domain can display synergistic and antagonistic interactions with the domains of the LBD.  
16 For example, studies with mutated and/or deleted receptors show positive cooperativity of the  
17 amino and carboxy terminal domains. In some cases, deletion of either of these domains will  
18 abolish the receptor's transcriptional activation functions.

### 19 20 *DNA-Binding Domain*

21 The DBD is the most conserved structure in the nuclear receptor superfamily. It  
22 usually contains about 70 amino acids that fold into two zinc finger motifs, wherein a zinc  
23 ion coordinates four cysteines. DBDs contain two perpendicularly oriented  $\alpha$ -helixes that  
24 extend from the base of the first and second zinc fingers. The two zinc fingers function in  
25 concert along with non-zinc finger residues to direct nuclear receptors to specific target sites  
26 on DNA and to align receptor homodimer or heterodimer interfaces. Various amino acids in  
27 DBD influence spacing between two half-sites (usually comprised of six nucleotides) for  
28 receptor dimer binding. For example, GR subfamily and ER homodimers bind to half-sites  
29 spaced by three nucleotides and oriented as palindromes. The optimal spacings facilitate  
30 cooperative interactions between DBDs, and D box residues are part of the dimerization



1 interface. Other regions of the DBD facilitate DNA-protein and protein-protein interactions  
2 required for RXR homodimerization and heterodimerization on direct repeat elements.

3 The LBD may influence the DNA binding of the DBD, and the influence can also be  
4 regulated by ligand binding. For example, TR ligand binding influences the degree to which  
5 a TR binds to DNA as a monomer or dimer. Such dimerization also depends on the spacing  
6 and orientation of the DNA half sites. The receptors also can interact with other proteins  
7 and function to regulate gene expression.

8 The nuclear receptor superfamily has been subdivided into two subfamilies: 1) GR  
9 (GR, AR, MR and PR) and 2) TR (TR, VDR, RAR, RXR, and most orphan receptors) on  
10 the basis of DBD structures, interactions with heat shock proteins (hsp), and ability to form  
11 heterodimers. GR subgroup members are tightly bound by hsp in the absence of ligand,  
12 dimerize following ligand binding and dissociation of hsp, and show homology in the DNA  
13 half sites to which they bind. These half sites also tend to be arranged as palindromes. TR  
14 subgroup members tend to be bound to DNA or other chromatin molecules when unliganded,  
15 can bind to DNA as monomers and dimers, but tend to form heterodimers, and bind DNA  
16 elements with a variety of orientations and spacings of the half sites, and also show  
17 homology with respect to the nucleotide sequences of the half sites. By this classification,  
18 ER does not belong to either subfamily, since it resembles the GR subfamily in hsp  
19 interactions, and the TR subfamily in nuclear localization and DNA-binding properties.

### 20 21 *Ligand Binding Domain*

22 The LBD is the second most highly conserved domain in these receptors. Whereas  
23 integrity of several different LBD sub-domains is important for ligand binding, truncated  
24 molecules containing only the LBD retain normal ligand-binding activity. This domain also  
25 participates in other functions, including dimerization, nuclear translocation and  
26 transcriptional activation, as described herein. Importantly, this domain binds the ligand and  
27 undergoes ligand-induced conformational changes as detailed herein.

28 Most members of the superfamily, including orphan receptors, possess at least two  
29 transcription activation subdomains, one of which is constitutive and resides in the amino  
30 terminal domain (AF-1), and the other of which (AF-2 (also referenced as TAU 4)) resides  
31 in the ligand-binding domain whose activity is regulated by binding of an agonist ligand.

1 The function of AF-2 requires an activation domain (also called transactivation domain) that  
2 is highly conserved among the receptor superfamily (approximately amino acids 1005 to  
3 1022). Most LBDs contain an activation domain. Some mutations in this domain abolish  
4 AF-2 function, but leave ligand binding and other functions unaffected. Ligand binding  
5 allows the activation domain to serve as an interaction site for essential co-activator proteins  
6 that function to stimulate (or in some cases, inhibit) transcription.

7 For example, Shibata, H., *et al.* (*Recent Progress in Hormone Res.* 52:141-164  
8 (1997)) has reviewed the role of co-activators and co-repressors in steroid/thyroid hormone  
9 receptor systems. Steroid receptor co-activator-one (SRC-1) appears to be a general co-  
10 activator for all AF-2 domain containing receptors tested. SRC-1 enhances transactivation of  
11 steroid hormone-dependent target genes. Other putative co-activators have been reported,  
12 including the SRC-1 related proteins, TIF-2 and GRIP-1, and other putative unrelated co-  
13 activators such as ARA-70, Trip 1, RIP-140, and TIF-1. In addition another co-activator  
14 CREB-binding protein (CBP) has been shown to enhance receptor-dependent target gene  
15 transcription. CBP and SRC-1 interact and synergistically enhance transcriptional activation  
16 by the ER and PR. A ternary complex of CBP, SRC-1, and liganded receptors may form to  
17 increase the rate of hormone-responsive gene transcription. Co-repressors, such as SMRT  
18 and N-CoR, for TR and RAR, have been identified that also contribute to the silencing  
19 function of unliganded TR. The unliganded TR and RAR have been shown to inhibit basal  
20 promoter activity; this silencing of target gene transcription by unliganded receptors is  
21 mediated by these co-repressors. The collective data suggests that upon binding of agonist,  
22 the receptor changes its conformation in the ligand-binding domain that enables recruitment  
23 of co-activators, which allows the receptor to interact with the basal transcriptional  
24 machinery more efficiently and to activate transcription. In contrast, binding of antagonists  
25 induces a different conformational change in the receptor. Although some antagonist-bound  
26 receptors can dimerize and bind to their cognate DNA elements, they fail to dislodge the  
27 associated co-repressors, which results in a nonproductive interaction with the basal  
28 transcriptional machinery. Similarly, the TR and RAR associate with co-repressors in the  
29 absence of ligand, thereby resulting in a negative interaction with the transcriptional  
30 machinery that silences target gene expression. In the case of mixed agonist/antagonists,  
31 such as 4-hydroxytamoxifen, activation of gene transcription may depend on the relative ratio

1 of co-activators and co-repressors in the cell or cell-specific factors that determine the  
2 relative agonistic or antagonistic potential of different compounds. These co-activators and  
3 co-repressors appear to act as an accelerator and/or a brake that modulates transcriptional  
4 regulation of hormone-responsive target gene expression.

5 The carboxy-terminal activation subdomain, as described herein is in close three  
6 dimensional proximity in the LBD to the ligand, so as to allow for ligands bound to the LBD  
7 to coordinate (or interact) with amino acid(s) in the activation subdomain. As described  
8 herein, the LBD of a nuclear receptor can be expressed, crystallized, its three dimensional  
9 structure determined with a ligand bound (either using crystal data from the same receptor or  
10 a different receptor or a combination thereof), and computational methods used to design  
11 ligands to its LBD, including ligands that contain an extension moiety that coordinates the  
12 activation domain of the nuclear receptor.

13 Once a computationally designed ligand (CDL) is synthesized as described herein and  
14 known in the art, it can be tested using assays to establish its activity as an agonist, partial -  
15 agonist or antagonist, and affinity, as described herein. After such testing, the CDLs can be  
16 further refined by generating LBD crystals with a CDL bound to the LBD. The structure of  
17 the CDL can then be further refined using the chemical modification methods described  
18 herein for three dimensional models to improve the activity or affinity of the CDL and make  
19 second generation CDLs with improved properties, such as that of a super agonist or  
20 antagonist described herein. Agonist and antagonist ligands also can be selected that  
21 modulate nuclear receptor responsive gene transcription through altering the interaction of  
22 co-activators and co-repressors with their cognate nuclear hormone receptor. For example,  
23 CDL agonists can be selected that block or dissociate the co-repressor from interaction with  
24 the receptor, and/or which promote binding or association of the co-activator. CDL  
25 antagonists can be selected that block co-activator interaction and/or promote co-repressor  
26 interaction with the target receptor. Selection can be done in binding assays that screen for  
27 CDLs having the desired agonist or antagonist properties. Suitable assays for such screening  
28 are described herein and in Shibata, H., *et al.* (*Recent Prog. Horm. Res.* 52:141-164  
29 (1997)); Tagami, T., *et al.* (*Mol. Cell Biol.* 17(5):2642-2648 (1997)); Zhu, XG., *et al.* (*J.*  
30 *Biol. Chem.* 272(14):9048-9054 (1997)); Lin, B.C., *et al.* (*Mol. Cell Biol.* 17(10):6131-6138  
31 (1997)); Kakizawa, T., *et al.* (*J. Biol. Chem.* 272(38):23799-23804 (1997)); and Chang, K.

1 H., *et al.* (*Proc. Natl. Acad. Sci. USA* 94(17):9040-9045 (1997)), which references are  
2 incorporated herein in their entirety by reference.

#### 4 NUCLEAR RECEPTOR ISOFORMS

5 The present invention also is applicable to generating new synthetic ligands to  
6 distinguish nuclear receptor isoforms. As described herein, CDLs can be generated that  
7 distinguish between binding isoforms, thereby allowing the generation of either tissue specific  
8 or function specific synthetic ligands. For instance, GR subfamily members have usually one  
9 receptor encoded by a single gene, although are exceptions. For example, there are two PR  
10 isoforms, A and B, translated from the same mRNA by alternate initiation from different  
11 AUG codons. There are two GR forms, one of which does not bind ligand. This method is  
12 especially applicable to the TR subfamily which usually has several receptors that are  
13 encoded by at least two (TR:  $\alpha$ ,  $\beta$ ) or three (RAR, RXR, and PPAR:  $\alpha$ ,  $\beta$ ,  $\gamma$ ) genes or have  
14 alternate RNA splicing and such an example for TR is described herein.

#### 16 NUCLEAR RECEPTOR CRYSTALS

17 The invention provides for crystals made from nuclear receptor ligand binding  
18 domains with the ligand bound to the receptor. As exemplified in the Examples, TRs are  
19 crystallized with a ligand bound to it. Crystals are made from purified nuclear receptor  
20 LBDs that are usually expressed by a cell culture, such as *E. coli*. Preferably, different  
21 crystals (co-crystals) for the same nuclear receptor are separately made using different  
22 ligands, such as a naturally occurring ligand and at least one bromo- or iodo- substituted  
23 synthetic ligand that acts as an analog or antagonist of the naturally occurring ligand. Such  
24 bromo- and iodo- substitutions act as heavy atom substitutions in nuclear receptor ligands and  
25 crystals of nuclear receptor proteins. This method has the advantage for phasing of the  
26 crystal in that it bypasses the need for obtaining traditional heavy metal derivatives. After  
27 the three dimensional structure is determined for the nuclear receptor LBD with its ligand  
28 bound, the three dimensional structure can be used in computational methods to design a  
29 synthetic ligand for the nuclear receptor and further activity structure relationships can be  
30 determined through routine testing using the assays described herein and known in the art.



## 1 *Expression and Purification of other Nuclear Receptor LBD Structures*

2 High level expression of nuclear receptor LBDs can be obtained by the techniques  
3 described herein as well as others described in the literature. High level expression in E.  
4 coli of ligand binding domains of TR and other nuclear receptors, including members of the  
5 steroid/thyroid receptor superfamily, such as the receptors ER, AR, MR, PR, RAR, RXR  
6 and VDR can also be achieved. Yeast and other eukaryotic expression systems can be used  
7 with nuclear receptors that bind heat shock proteins as these nuclear receptors are generally  
8 more difficult to express in bacteria, with the exception of ER, which can be expressed in  
9 bacteria. Representative nuclear receptors or their ligand binding domains have been cloned  
10 and sequenced: human RAR- $\alpha$ , human RAR- $\gamma$ , human RXR- $\alpha$ , human RXR- $\beta$ , human  
11 PPAR- $\alpha$ , human PPAR- $\beta$ , human PPAR- $\gamma$ , human VDR, human ER (as described in  
12 Seielstad *et al.*, *Molecular Endocrinology*, vol 9:647-658 (1995), incorporated herein by  
13 reference), human GR, human PR, human MR, and human AR. The ligand binding domain  
14 of each of these nuclear receptors has been identified and is shown in FIG. 3. Using the  
15 information in FIG. 3 in conjunction with the methods described herein and known in the  
16 art, one of ordinary skill in the art could express and purify LBDs of any of the nuclear  
17 receptors, including those illustrated in FIG. 3, bind it to an appropriate ligand, and  
18 crystallize the nuclear receptor's LBD with a bound ligand.

19 FIG. 3 is an alignment of several members of the steroid/thyroid hormone receptor  
20 superfamily that indicates the amino acids to be included in a suitable expression vector.

21 Extracts of expressing cells are a suitable source of receptor for purification and  
22 preparation of crystals of the chosen receptor. To obtain such expression, a vector is  
23 constructed in a manner similar to that employed for expression of the rat TR alpha (Apriletti  
24 *et al.* *Protein Expression and Purification*, 6:363-370 (1995), herein incorporated by  
25 reference). The nucleotides encoding the amino acids encompassing the ligand binding  
26 domain of the receptor to be expressed, for example the estrogen receptor ligand binding  
27 domain (hER-LBD) (corresponding to R at position 725 to L at position 1025 as standardly  
28 aligned as shown in the FIG. 3), are inserted into an expression vector such as the one  
29 employed by Apriletti *et al.* (1995). For the purposes of obtaining material that will yield  
30 good crystals it is preferable to include at least the amino acids corresponding to human TR-  
31  $\beta$  positions 725 to 1025. Stretches of adjacent amino acid sequences may be included if

1 more structural information is desired. Thus, an expression vector for the human estrogen  
2 receptor can be made by inserting nucleotides encoding amino acids from position 700 to the  
3 c-terminus at position 1071. Such a vector gives high yield of receptor in *E. coli* that can  
4 bind hormone (Seielstad *et al. Molecular Endocrinology* 9:647-658 (1995)). However, the c-  
5 terminal region beyond position 1025 is subject to variable proteolysis and can  
6 advantageously be excluded from the construct, this technique of avoiding variable  
7 proteolysis can also be applied to other nuclear receptors.

### 9 *TR- $\alpha$ And TR- $\beta$ As Examples of Nuclear receptor LBD Structure and Function*

#### 10 *TR Expression, Purification And Crystallization*

11 As an example of nuclear receptor structure of the ligand binding domain the  $\alpha$ - and  
12  $\beta$ - isoforms of TR are crystallized from proteins expressed from expression constructs,  
13 preferably constructs that can be expressed in *E. coli*. Other expression systems, such as  
14 yeast or other eukaryotic expression systems can be used. For the TR, the LBD can be  
15 expressed without any portion of the DBD or amino-terminal domain. Portions of the DBD  
16 or amino-terminus can be included if further structural information with amino acids adjacent  
17 the LBD is desired. Generally, for the TR the LBD used for crystals will be less than 300  
18 amino acids in length. Preferably, the TR LBD will be at least 150 amino acids in length,  
19 more preferably at least 200 amino acids in length, and most preferably at least 250 amino  
20 acids in length. For example the LBD used for crystallization can comprise amino acids  
21 spanning from Met 122 to Val 410 of the rat TR- $\alpha$ , Glu 202 to Asp 461 of the human TR- $\beta$ .

22 Typically TR LBDs are purified to homogeneity for crystallization. Purity of TR  
23 LBDs is measured with sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-  
24 PAGE), mass spectrometry (MS) and hydrophobic high performance liquid chromatography  
25 (HPLC). The purified TR for crystallization should be at least 97.5 % pure or 97.5%,  
26 preferably at least 99.0% pure or 99.0% pure, more preferably at least 99.5% pure or  
27 99.5% pure.

28 Initially purification of the unliganded receptor can be obtained by conventional  
29 techniques, such as hydrophobic interaction chromatography (HPLC), ion exchange  
30 chromatography (HPLC), and heparin affinity chromatography.



1 To achieve higher purification for improved crystals of nuclear receptors, especially  
2 the TR subfamily and TR, it will be desirable to ligand shift purify the nuclear receptor using  
3 a column that separates the receptor according to charge, such as an ion exchange or  
4 hydrophobic interaction column, and then bind the eluted receptor with a ligand, especially  
5 an agonist. The ligand induces a change in the receptor's surface charge such that when re-  
6 chromatographed on the same column, the receptor then elutes at the position of the liganded  
7 receptor are removed by the original column run with the unliganded receptor. Usually  
8 saturating concentrations of ligand are used in the column and the protein can be  
9 preincubated with the ligand prior to passing it over the column. The structural studies  
10 detailed herein indicate the general applicability of this technique for obtaining super-pure  
11 nuclear receptor LBDs for crystallization.

12 More recently developed methods involve engineering a "tag" such as with histidine  
13 placed on the end of the protein, such as on the amino terminus, and then using a nickle  
14 chelation column for purification, Janknecht R., *Proc. Natl. Acad. Sci. USA*, 88:8972-8976-  
15 (1991) incorporated by reference.

16 To determine the three dimensional structure of a TR LBD, or a LBD from another  
17 member of the nuclear receptor superfamily, it is desirable to co-crystallize the LBD with a  
18 corresponding LBD ligand. In the case of TR LBD, it is preferable to separately co-  
19 crystallize it with ligands such as T3, IpBr and Dimit that differ in the heavy atoms which  
20 they contain. Other TR ligands such as those encompassed by Formula 1 described herein  
21 and known in the prior art, can also be used for the generation of co-crystals of TR LBD and  
22 TR ligands. Of the compounds encompassed by Formula 1 it is generally desirable to use at  
23 least one ligand that has at least one bromo- or iodo- substitution at the  $R_3$ ,  $R_5$ ,  $R_3'$  or  $R_5'$   
24 position, preferably such compounds will be have at least two such substitutions and more  
25 preferably at least 3 such substitutions. As described herein, such substitutions are  
26 advantageously used as heavy atoms to help solve the phase problem for the three  
27 dimensional structure of the TR LBD and can be used as a generalized method of phasing  
28 using a halogen (e.g. I or Br) substituted ligand, especially for nuclear receptors.

29 Typically purified LBD, such as TR LBD, is equilibrated at a saturating concentration  
30 of ligand at a temperature that preserves the integrity of the protein. Ligand equilibration

1 can be established between 2 and 37°C, although the receptor tends to be more stable in the  
2 2-20°C range.

3 Preferably crystals are made with the hanging drop methods detailed herein.  
4 Regulated temperature control is desirable to improve crystal stability and quality.  
5 Temperatures between 4 and 25°C are generally used and it is often preferable to test  
6 crystallization over a range of temperatures. In the case of TR it is preferable to use  
7 crystallization temperatures from 18 to 25°C, more preferably 20 to 23°C, and most  
8 preferably 22°C.

9 Complexes of the TR- $\alpha$  LBD with a variety of agonists, including T<sub>3</sub>, IpBr<sub>2</sub>, Dimit,  
10 and Triac, are prepared with by methods described herein. For example, cocrystals of the  
11 rTR- $\alpha$  LBD, with ligand prebound, are prepared by vapor diffusion at ambient temperature  
12 from 15% 2-methyl-2,4-pentanediol (MPD). The crystals are radiation sensitive, and require  
13 freezing to measure complete diffraction data. On a rotating anode X-ray source, the  
14 crystals diffract to  $\sim 3\text{\AA}$ ; synchrotron radiation extends the resolution limit significantly, to -  
15 as high as 2.0 $\text{\AA}$  for T<sub>3</sub> cocrystals. The composition of the thyroid hormone, combined with  
16 the ability to prepare and cocrystallize the receptor complexed with a variety of analogs,  
17 permitted the unusual phasing strategy. This phasing strategy can be applied to the ligands  
18 of the nuclear receptors described therein by generating I and Br substitutions of such  
19 ligands. In this strategy, cocrystals of the TR LBD containing four hormone analogs that  
20 differ at the 3,5, and 3' positions (T<sub>3</sub>, IpBr<sub>2</sub>, Dimit, and Triac) provided isomorphous  
21 derivatives. For this set of analogs, the halogen substituents (2Br and 3I atoms) function as  
22 heavy atoms, while the Dimit cocrystal (3 alkyl groups) acts as the parent. The initial 2.5 $\text{\AA}$   
23 multiple isomorphous replacement/anomalous scattering/density modified electron density  
24 map allowed the LBD to be traced from skeletons created in the molecular graphics program  
25 O5 (Jones, T.A. *et al.*, *ACTA Cryst*, 47:110-119 (1991), incorporated by reference herein).  
26 A model of the LBD was built in four fragments, Arg157-Gly184, Trp186-Gly197, Ser199-  
27 Pro205, and Val210-Phe405, and refined in XPLOR using positional refinement and  
28 simulated annealing protocols. Missing residues were built with the aid of difference  
29 density. The final model was refined to  $R_{\text{cryst}} = 21.8\%$  and  $R_{\text{free}} = 24.4\%$  for data from  
30 15.0 to 2.2 $\text{\AA}$ , see Table 6. The human TR- $\beta$  LBD model was resolved by molecular  
31 replacement of the TR- $\alpha$  LBD coordinates. The structure is based on E202 to D461 with a

1 his-tag at the N-terminus. The final model was refined to  $R_{\text{cryst}} = 25.3\%$  and  $R_{\text{free}} = 28.9\%$   
2 for data from 30.0 to 2.4Å+, see Table 7.

3 This phasing strategy can be applied to the ligands of the nuclear receptors described  
4 herein by generating I and Br substitutions of such ligands.

## 6 THREE DIMENSIONAL STRUCTURE OF TR LBD

### 7 *Architecture of TR LBD*

8 As an example of the three dimensional structure of a nuclear receptor, the folding of  
9 the TR- $\alpha_1$  LBD is shown in FIG. 4. The TR- $\alpha$  LBD consists of a single structural domain  
10 packed in three layers, composed of twelve  $\alpha$ -helices, H1-12, and four short  $\beta$ -strands, S1-4,  
11 forming a mixed  $\beta$ -sheet. The buried hormone and three antiparallel  $\alpha$ -helices, H5-6, H9,  
12 and H10, form the central layer of the domain, as shown in FIG. 4. H1, H2, H3 and S1  
13 form one face of the LBD, with the opposite face formed by H7, H8, H11, and H12. The  
14 first 35 amino acids of the N-terminus (Met122-Gln156) are not visible in the electron  
15 density maps. The three dimensional structure of the heterodimeric RXR:TR DNA-binding  
16 domains bound to DNA, amino acids Met 122 - Gln151 of the TR DBD make extensive  
17 contacts with the minor groove of the DNA8. The five disordered amino acids (Arg152-  
18 Gln156), which reside between the last visible residue of the TR DBD and the first visible  
19 residue of the LBD likely represent the effective "hinge" linking the LBD and the DBD in  
20 the intact receptor.

21 The predominantly helical composition and the layered arrangement of secondary  
22 structure is identical to that of the unliganded hRXR $\alpha$ , confirming the existence of a common  
23 nuclear receptor fold between two nuclear receptors.

24 The TR LBD is visible beginning at Arg157, and continues in an extended coil  
25 conformation to the start of H1. A turn of  $\alpha$ -helix, H2, covers the hormone binding cavity,  
26 immediately followed by short  $\beta$ -strand, S1, which forms the edge of the mixed  $\beta$ -sheet,  
27 parallel to S4, the outermost of the three antiparallel strands. The chain is mostly irregular  
28 until H3 begins, antiparallel to H1. H3 bends at Ile221 and Ile222, residues which contact  
29 the ligand. The chain turns almost 90° at the end of H3 to form an incomplete  $\alpha$ -helix, H4.  
30 The first buried core helix, H5-6, follows, its axis altered by a kink near the ligand at Gly  
31 253. The helix is composed of mostly hydrophobic sidechains interrupted by two striking

exceptions: Arg262 is solvent inaccessible and interacts with the ligand carboxylate (1-  
 substituent), and Glu256 meets Arg329 from H9 and Arg375 from H11 in a polar  
 invagination. H5-6 terminates in a short  $\beta$ -strand, S2, of the four strand mixed sheet. S3  
 and S4 are joined through a left-handed turn, and further linked by a salt bridge between  
 Lys284 and Asp272. Following S4, H7 and H8 form an L, stabilized by a salt bridge  
 between Lys268 and Asp277. The turn between H7 and H8 adopts an unusual conformation,  
 a result of interaction with ligand and its glycine rich sequence. H9 is the second core helix.  
 antiparallel to the neighboring H5-6. Again, two buried polar sidechains are found, Glu315  
 and Gln320. Glu315 forms a buried salt bridge with His358 and Arg356. The oxygen of  
 Gln320 forms a hydrogen bond with the buried sidechain of His 175. The chain then  
 switches back again to form H10, also antiparallel to H9. H11 extends diagonally across the  
 full length of the molecule. Immediately after H11, the chain forms a type II turn, at  
 approximately 90° to H11. The chain then turns again to form H 12, which packs loosely  
 against H3 and H11 as part of the hormone or ligand binding cavity. The final five amino -  
 acids at the C-terminus, Glu406 -Val410, are disordered. The architecture of the TR- $\beta$  LBD  
 is identical to that of the TR- $\alpha$  LBD, with two significant differences. An additional helix is  
 present at the N-terminus (residues Glu202-Ile208), which is part of the DBD, and packs  
 antiparallel to H10. Following the helix is a two residue turn (Gly209-His210) continuing  
 into an extended coil to the start of H1, as seen in the TR- $\alpha$  LBD. A further difference  
 occurs in the irregular conformation adopted between H2 and H3. In the TR- $\alpha$  LBD,  
 residue Gly197-Asp211 form a loop that packs against the receptor, contacting helices H7,  
 H8, H11, and the loop between H11 and H12. In the TR- $\beta$  LBD, only the ends of the loop  
 are ordered, with the stretch Ala253-Lys263 disordered. In addition to these residues, the  
 residues of the His-tag at the N-terminus, and the final residue at the C-terminus, Asp461,  
 are disordered.

## *TR LBD's Ligand Binding Cavity As An Example Of A Nuclear Receptor's Buried Ligand Cavity*

The three dimensional structure of the TR LBD leads to the startling finding that  
 ligand binding cavity of the LBD is solvent inaccessible when a T3 or its isostere is bound to  
 the LBD. This surprising result leads to a new model of nuclear receptor three dimensional



1 structure and function, as further described herein, particularly in the sections elucidating the  
2 computational methods of ligand design and the application of such methods to designing  
3 nuclear receptor synthetic ligands that contain extended positions that prevent normal  
4 activation of the activation domain.

5 Dimit, the ligand bound to the receptor, is an isostere of  $T_3$  and a thyroid hormone  
6 agonist. Therefore the binding of Dimit should reflect that of  $T_3$ , and the Dimit-bound  
7 receptor is expected to be the active conformation of TR. The ligand is buried within the  
8 receptor, providing the hydrophobic core for a subdomain of the protein, as shown in FIG. 5  
9 a and b. H5-6 and H9 comprise the hydrophobic core for the rest of the receptor.

10 An extensive binding cavity is constructed from several structural elements. The  
11 cavity is enclosed from above by H5-6 (Met 256- Arg266), from below by H7 and H8 and  
12 the intervening loop (Leu287- Ile299), and along the sides by H2 (185-187), by the turn  
13 between S3 and S4 (Leu276-Ser277), by H3 (Phe215-Arg228), by H11 (His381-Met388) and  
14 by H12 (Phe401-Phe405). The volume of the cavity defined by these elements, calculated by  
15 GRASP (Columbia University, USA) (600 Å<sup>3</sup>), is essentially the volume of the hormone  
16 (530 Å<sup>3</sup>). The change in volume can be exploited for ligand design as described herein. The  
17 remaining volume is occupied by water molecules surrounding the amino-propionic acid  
18 substituent. FIG. 6 depicts various contacts (or interactions) between TR's LBD and the  
19 ligand.

20 The planes of the inner and outer (prime ring) rings of the ligand are rotated from  
21 planarity about 60° with respect to each other, adopting the 3'-distal conformation (in which  
22 the 3' substituent of the outer ring projects down and away from the inner ring). The amino-  
23 propionic acid and the outer phenolic ring assume the transoid conformation, each on  
24 opposite sides of the inner ring. The torsion angle  $\chi_1$  for the amino- propionic acid is 300°.

25 The amino-propionic acid substituent is packed loosely in a polar pocket formed by  
26 side chains from H2, H4 and S3. The carboxylate group forms direct hydrogen bonds with  
27 the guanidium group of Arg228 and the amino N of Ser277. In addition, Arg262, Arg266  
28 and Asn179 interact with the carboxylate through water-mediated hydrogen bonds. The three  
29 arginine residues create a significantly positive local electrostatic potential, which may  
30 stabilize the negative charge of the carboxylate. No hydrogen bond is formed by the amino  
31 nitrogen. The interactions of the amino-propionic acid substituent are consistent with the fact

1 that Triac, which lacks the amino nitrogen, has a binding affinity equal to that of  $T_3$ ,  
2 indicating that the amino nitrogen and longer aliphatic chain of  $T_3$  do not contribute greatly to  
3 binding affinity.

4 The biphenyl ether, in contrast, is found buried within the hydrophobic core. The  
5 inner ring packs in a hydrophobic pocket formed by H3, H5-6, and S3. Pockets for the 3-  
6 and 5-methyl substituents are not completely filled, as expected since the van der Waals  
7 radius of methyl substituent for Dimit is smaller than the iodine substituent provided by the  
8 thyroid hormone  $T_3$ . Such pockets are typically 25 to 100 cubic angstroms (although smaller  
9 pocket for substitutes are contemplated in the 40 to 80 cubic angstrom range) and could be  
10 filled more tightly with better fitting chemical substitutions, as described herein.

11 The outer ring packed tightly in a pocket formed by H3, H5-6, H7, H8, H11 and  
12 H12, and the loop between H7 and H8. The ether oxygen is found in a hydrophobic  
13 environment defined by Phe218, Leu287, Leu276, and Leu292. The absence of a hydrogen  
14 bond to the ether oxygen is consistent with its role in establishing the correct stereochemistry  
15 of the phenyl rings, as suggested by potent binding of hormone analogs with structurally  
16 similar linkages possessing reduced or negligible hydrogen bonding capability. The 3'-  
17 isopropyl substituent contacts Gly290 and 291. The presence of glycine at this position in  
18 the pocket can explain the observed relationship between activity and the size of 3'-  
19 substituents. Activity is highest for 3'-isopropyl, and decreases with added bulk. The only  
20 hydrogen bond in the hydrophobic cavity is formed between the phenolic hydroxyl and  
21 His381 N $\epsilon$ 2. The conformation of His381 is stabilized by packing contacts provided by  
22 Phe405, and Met256.

23 The presence of a 5' substituent larger than hydrogen affects the binding affinity for  
24 hormone. The more abundant thyroid hormone, 3,5,3',5'-tetraiodo-L-thyronine ( $T_4$ ), contains  
25 an iodine at this position, and binds the receptor with 2% of the affinity of  $T_3$ . The structure  
26 suggests that discrimination against  $T_4$  is accomplished through the combination of steric  
27 conflict by Met256 and possibly the constraints imposed by the geometry of the hydrogen  
28 bond from His381 to the phenolic hydroxyl. The 5' position is a preferred location for  
29 introducing a chemical modification of C-H at the 5' of  $T_3$  or and TR agonist, as described  
30 herein, that produces an extension from the prime ring and results in the creation of an  
31 antagonist or partial agonist.



1 Deletion and antibody competition studies suggest the involvement of residues Pro162  
2 to Val202 in ligand binding. The region does not directly contact hormone in the bound  
3 structure, although H2 packs against residues forming the polar pocket that interacts with the  
4 amino-propionic acid group. One role for H2, then, is to stabilize these residues in the bound  
5 state, H2, with  $\beta$ -strands S3 and S4, might also represent a prevalent entry point for ligand,  
6 since the amino-propionic acid of the ligand is oriented toward this region. Studies of  
7 receptor binding to  $T_3$  affinity matrices demonstrate that only a linkage to the amino-  
8 propionic acid is tolerated, suggesting that steric hindrance present in other linkages prevent  
9 binding. Furthermore, the crystallographic temperature factors suggest the coil and  $\beta$ -strand  
10 region is most flexible part of the domain FIG. 7. Participation of this region, part of the  
11 hinge domain between the DBD and LBD, in binding hormone may provide structural means  
12 for ligand binding to influence DNA binding, since parts of the Hinge domain contact DNA.

### 13 14 *TR LBD Transcriptional Activation Helix As An Example Of A Nuclear Receptor* 15 *Activation Domain*

16 In addition to the startling finding that the ligand binding cavity is solvent inaccessible  
17 when loaded with a ligand, the activation helix of TR LBD presents a surface to the ligand  
18 cavity for interaction between at least one amino acid and the bound ligand. The C-terminal  
19 17 amino acids of the TR, referred to as the activation helix or AF-2 (an example of an LBD  
20 activation domain), are implicated in mediating hormone-dependent transcriptional activation.  
21 Although, mutations of key residues within the domain decrease ligand-dependent activation  
22 it was unclear until the present invention whether such mutations directly affected ligand  
23 coordination. Although some mutations of this domain have been noted to reduce or abolish  
24 ligand binding, other mutations in more distant sites of the LBD have a similar effect.

25 Activation domains among nuclear receptors display an analogous three dimensional  
26 relationship to the binding cavity, which is a region of the LBD that binds the molecular  
27 recognition domain of a ligand, i.e. the activation domain presents a portion of itself to the  
28 binding cavity (but necessarily the molecular recognition domain of the ligand). Many  
29 nuclear receptors are expected to have such domains, including the retinoid receptors, RAR  
30 and RXR, the glucocorticoid receptor GR, and the estrogen receptor ER. Based upon the  
31 TR's sequence, the domain is proposed to adopt an amphipathic helical structure.  $\beta$ -sheet or

1 mixed secondary structures, could be present as activation domains in less related nuclear  
2 receptors.

3       Within the activation domain, the highly conserved motif  $\Phi\Phi X E \Phi\Phi$ , where  $\Phi$   
4 represents a hydrophobic residue, is proposed to mediate interactions between the receptors  
5 and transcriptional coactivators. Several proteins have been identified which bind the TR in  
6 a hormone-dependent fashion. One of these, Trip1, is related to a putative yeast coactivator  
7 Sug1, and also interacts with both the C-terminal activation domain and a subset of the basal  
8 transcriptional machinery, suggesting a role in transactivation by the TR. Other proteins,  
9 such as RIP140, SRC1, (Onate, S.A. et. al., *Science* 270:1354-1357 (1995)) and TF-1 (see  
10 also Ledouarim, B., et. al., *EMBO J.* 14:2020-2033 (1995)), and GRIP-1 (Heery, E., et al.,  
11 *Nature* 387:733-736 (1997)) also interact with other nuclear receptors in a ligand dependent  
12 manner through the C-terminal domain. Binding of these proteins can be modulated using  
13 the TR ligands described herein especially those TR ligands with extensions that sterically  
14 hinder the interaction between the highly conserved motif and other proteins.

15       The C-terminal activation domain of the TR forms an amphipathic helix, H12, which  
16 nestles loosely against the receptor to form part of the hormone binding cavity. The helix  
17 packs with the hydrophobic residues facing inward towards the hormone binding cavity, and  
18 the charged residues, including the highly-conserved glutamate, extending into the solvent, as  
19 shown in FIG. 8. The activation helix of TR LBD presents Phe 401 to the ligand binding  
20 cavity and permits direct coordination with the hormone i.e. such amino acids interact with  
21 the ligand forming a van der waals contact with the plane of the outer phenyl ring. Phe 405  
22 also interacts with His 381, perhaps stabilizing its hydrogen bonding conformation, i.e. a  
23 favorable hydrogen bond interaction. Participation of Phe 401 and Phe 405 in binding  
24 hormone explains how mutation of these residues decreases hormone binding affinity.  
25 Furthermore, the impact of these mutations on activation likely derives from a role in  
26 stabilizing the domain in the bound structure through increased hydrogen bond interaction of  
27 dipole interactions. Glu 403 extends into the solvent, emphasizing its critical role in  
28 transactivation. In its observed conformation, presented on the surface as an ordered  
29 residue, against a background of predominantly hydrophobic surface, Glu 403 is available to  
30 interact with activator proteins described herein, as shown in FIG. 9. The other charged  
31 residues, Glu 405 and Asp 406 are disordered, as the helix frays at Phe 405.

Two other sequences in the TR,  $\tau 2$  and  $\tau 3$ , activate transcription when expressed as fusion proteins with a DNA-binding domain. The sequences, discovered in the TRB, correspond to TR- $\alpha$  residues Pro158-Ile168 in H1 ( $\tau 2$ ), and Gly290-Leu319 in H8 and H9 ( $\tau 3$ ). Unlike the C-terminal activation domain,  $\tau 2$  and  $\tau 3$  do not appear to represent modular structural units in the rat TR- $\alpha$  LBD, nor present a surface for protein-protein interactions: the critical aspartate/glutamate residues of  $\tau 3$  are located on two separate helices, and do not form a single surface; the charged residues of  $\tau 2$  are engaged in ion pair interactions with residues of the LBD. Thus,  $\tau 2$  and  $\tau 3$  may not function as activation domains in the context of the entire receptor.

### Computational Methods For Designing A Nuclear Receptor LBD LIGAND

The elucidation of the three dimensional structure of a nuclear receptor ligand binding domain provides an important and useful approach for designing ligands to nuclear receptors using the computational methods described herein. By inspecting the **FIGURES** it can be determined that the nuclear receptor ligand is bound in a water inaccessible binding cavity in the LBD and that chemical moieties can be added to selected positions on the ligand. Such chemical modifications, usually extensions, can fill up the binding cavity represented in the **FIGURES** for a tighter fit (or less water) or can be used to disrupt or make contacts with amino acids not in contact with the ligand before the chemical modification was introduced or represented in a figure of the three dimensional model of the LBD. Ligands that interact with nuclear superfamily members can act as agonists, antagonists and partial agonists based on what ligand-induced conformational changes take place.

Agonists induce changes in receptors that place them in an active conformation that allows them to influence transcription, either positively or negatively. There may be several different ligand-induced changes in the receptor's conformation.

Antagonists, bind to receptors, but fail to induce conformational changes that alter the receptor's transcriptional regulatory properties or physiologically relevant conformations. Binding of an antagonist can also block the binding and therefore the actions of an agonist.

Partial agonists bind to receptors and induce only part of the changes in the receptors that are induced by agonists. The differences can be qualitative or quantitative. Thus, a

1 partial agonist may induce some of the conformation changes induced by agonists, but not  
2 others, or it may only induce certain changes to a limited extent.

### 4 **Ligand-induced Conformational Changes**

5 As described herein, the unliganded receptor is in a configuration that is either  
6 inactive, has some activity or has repressor activity. Binding of agonist ligands induces  
7 conformational changes in the receptor such that the receptor becomes more active, either to  
8 stimulate or repress the expression of genes. The receptors may also have non-genomic  
9 actions. Some of the known types of changes and/or the sequelae of these are listed herein.

### 11 ***Heat Shock Protein Binding***

12 For many of the nuclear receptors ligand binding induces a dissociation of heat shock  
13 proteins such that the receptors can form dimers in most cases, after which the receptors  
14 bind to DNA and regulate transcription.

15 Nuclear receptors usually have heat shock protein binding domains that present a  
16 region for binding to the LBD and can be modulated by the binding of a ligand to the LBD.  
17 Consequently, an extended chemical moiety (or more) from the ligand that stabilizes the  
18 binding or contact of the heat shock protein binding domain with the LBD can be designed  
19 using the computational methods described herein to produce a partial agonist or antagonist.  
20 Typically such extended chemical moieties will extend past and away from the molecular  
21 recognition domain on the ligand and usually past the buried binding cavity of the ligand.

### 23 ***Dimerization and Heterodimerization***

24 With the receptors that are associated with the hsp in the absence of the ligand,  
25 dissociation of the hsp results in dimerization of the receptors. Dimerization is due to  
26 receptor domains in both the DBD and the LBD. Although the main stimulus for  
27 dimerization is dissociation of the hsp, the ligand-induced conformational changes in the  
28 receptors may have an additional facilitative influence. With the receptors that are not  
29 associated with hsp in the absence of the ligand, particularly with the TR, ligand binding can  
30 affect the pattern of dimerization/heterodimerization. The influence depends on the DNA  
31 binding site context, and may also depend on the promoter context with respect to other



1 proteins that may interact with the receptors. A common pattern is to discourage monomer  
2 formation, with a resulting preference for heterodimer formation over dimer formation on  
3 DNA.

4 Nuclear receptor LBDs usually have dimerization domains that present a region for  
5 binding to another nuclear receptor and can be modulated by the binding of a ligand to the  
6 LBD. Consequently, an extended chemical moiety (or more) from the ligand that disrupts  
7 the binding or contact of the dimerization domain can be designed using the computational  
8 methods described herein to produce a partial agonist or antagonist. Typically such extended  
9 chemical moieties will extend past and away from the molecular recognition domain on the  
10 ligand and usually past the buried binding cavity of the ligand.

11

## 12 *DNA Binding*

13 In nuclear receptors that bind to hsp, the ligand-induced dissociation of hsp with  
14 consequent dimer formation allows, and therefore, promotes DNA binding. With receptors  
15 that are not associated (as in the absence of ligand), ligand binding tends to stimulate DNA  
16 binding of heterodimers and dimers, and to discourage monomer binding to DNA.  
17 However, ligand binding to TR, for example, tends to decrease dimer binding on certain  
18 DNA elements and has minimal to no effect on increasing heterodimer binding. With DNA  
19 containing only a single half site, the ligand tends to stimulate the receptor's binding to  
20 DNA. The effects are modest and depend on the nature of the DNA site and probably on the  
21 presence of other proteins that may interact with the receptors. Nuclear receptors usually  
22 have DBDs that present a region for binding to DNA and this binding can be modulated by  
23 the binding of a ligand to the LBD. Consequently, an extended chemical moiety (or more)  
24 from the ligand that disrupts the binding or contact of the DBD can be designed using the  
25 computational methods described herein to produce a partial agonist or antagonist. Typically  
26 such extended chemical moieties will extend past and away from the molecular recognition  
27 domain on the ligand and usually past the buried binding cavity of the ligand.

28

## 29 *Repressor Binding*

30 Receptors that are not associated with hsp in the absence of ligand frequently act as  
31 transcriptional repressors in the absence of the ligand. This appears to be due, in part, to

1 transcriptional repressor proteins that bind to the LBD of the receptors. Agonist binding  
2 induces a dissociation of these proteins from the receptors. This relieves the inhibition of  
3 transcription and allows the transcriptional transactivation functions of the receptors to  
4 become manifest.

5

### 6 *Transcriptional Transactivation Functions*

7 Ligand binding induces transcriptional activation functions in two basic ways. The  
8 first is through dissociation of the hsp from receptors. This dissociation, with consequent  
9 dimerization of the receptors and their binding to DNA or other proteins in the nuclear  
10 chromatin allows transcriptional regulatory properties of the receptors to be manifest. This  
11 may be especially true of such functions on the amino terminus of the receptors.

12 The second way is to alter the receptor to interact with other proteins involved in  
13 transcription. These could be proteins that interact directly or indirectly with elements of the  
14 proximal promoter or proteins of the proximal promoter. Alternatively, the interactions  
15 could be through other transcription factors that themselves interact directly or indirectly with  
16 proteins of the proximal promoter. Several different proteins have been described that bind  
17 to the receptors in a ligand-dependent manner. In addition, it is possible that in some cases,  
18 the ligand-induced conformational changes do not affect the binding of other proteins to the  
19 receptor, but do affect their abilities to regulate transcription.

20 Nuclear receptors or nuclear receptor LBDs usually have activation domains  
21 modulated in part by a co-activator/co-repressor system that coordinately functions to present  
22 a region for binding to DNA, and can be modulated by the binding of a ligand to the LBD.  
23 Consequently, an extended chemical moiety (or more) from the ligand that disrupts the  
24 binding or contact of the activation domain with co-activator and/or co-repressor can be  
25 designed using the computational methods described herein to produce a partial agonist or  
26 antagonist. For instance, an agonist can be designed and/or selected which (1) blocks  
27 binding and/or dissociates co-repressor, and/or (2) promotes binding and/or association of a  
28 co-activator. An antagonist can be designed which (1) promotes binding and/or association  
29 of co-repressor, and/or (2) promotes binding and/or association of co-activator. Ratios of  
30 agonists and antagonists may be used to modulate transcription of the gene of interest.  
31 Selection can be accomplished in binding assays that screen for ligands having the desired



agonist or antagonist properties, including such ligands which induce conformational changes as described below. Suitable assays for such screening are described herein and in Shibata, H., *et al.* (*Recent Prog. Horm. Res.* 52:141-164 (1997)); Tagami, T., *et al.* (*Mol. Cell Biol.* 17(5):2642-2648 (1997)); Zhu, XG., *et al.* (*J. Biol. Chem.* 272(14):9048-9054 (1997)); Lin, B.C., *et al.* (*Mol. Cell Biol.* 17(10):6131-6138 (1997)); Kakizawa, T., *et al.* (*J. Biol. Chem.* 272(38):23799-23804 (1997)); and Chang, K. H., *et al.* (*Proc. Natl. Acad. Sci. USA* 94(17):9040-9045 (1997)). Typically such extended chemical moieties will extend past and away from the molecular recognition domain on the ligand and usually past the buried binding cavity of the ligand and in the direction of the activation domain, which is often a helix as seen in the three dimensional model shown in the **FIGURES** in two dimensions on paper or more conveniently on a computer screen.

### **Ligand-Induced Conformational Change**

Plasma proteins bind hormones without undergoing a conformational change through a static binding pocket formed between monomers or domains. For example, the tetrameric thyroid-binding plasma protein transthyretin forms a solvent-accessible hormone-binding channel at the oligomer interface. The structure of the protein is unchanged upon binding hormone with respect to the appearance of a buried binding cavity with a ligand bound.

However, the structural role for a ligand bound to a nuclear receptor LBD, like rat TR- $\alpha$  LBD, predicts that the receptor would differ in the bound and unbound states. In the absence of hormone, the receptor would possess a cavity at its core, uncharacteristic of a globular protein. A ligand (e.g. hormone) completes the hydrophobic core of the active receptor after it binds to the nuclear receptor. Ligand binding by the receptor is a dynamic process, which regulates receptor function by inducing an altered conformation.

An exact description of the hormone-induced conformational changes requires comparison of the structures of the liganded and the unliganded TR. The structure of the unliganded human RXR $\alpha$  may substitute as a model for the unliganded TR. The rat TR- $\alpha$  LBD and human RXR $\alpha$  LBDs adopt a similar fold, and it is likely that the structural similarity extends to the conformational changes after ligand binding.

There are three major differences between the two structures, which indeed appear to be the result of ligand binding. First, the bound rat TR- $\alpha$  LBD structure is more compact,

1 with the hormone tightly packed within the hydrophobic core of the receptor. By contrast,  
2 the unliganded human RXR $\alpha$  LBD contains several internal hydrophobic cavities. The  
3 presence of such cavities is unusual in folded proteins, and is likely a reflection of the  
4 unliganded state of the receptor. Two of these cavities were proposed as possible binding  
5 sites for 9-cis retinoic acid, though these multiple sites only partly overlap with the single  
6 buried binding cavity observed in the liganded rat TR- $\alpha$  LBD.

7 The second difference involves H11 in the rat TR- $\alpha$  LBD, which contributes part of  
8 the hormone binding cavity. H11, continuous in the rat TR- $\alpha$  LBD, is broken at Cys 432 in  
9 the RXR, forming a loop between H10 and H11 in the hRXR $\alpha$ . This residue corresponds to  
10 His381 in the TR, which provides a hydrogen bond to the outer ring hydroxyl of the ligand.  
11 Furthermore, the hormone binding cavity occupied by ligand in the rat TR- $\alpha$  LBD is  
12 interrupted in the hRXR $\alpha$  by the same loop, forming an isolated hydrophobic pocket in the  
13 RXR with H6 and H7. In the bound rat TR- $\alpha$  LBD, the corresponding helices H7 and H8  
14 are contiguous with the binding pocket, and enclose the hormone binding cavity from below.

15 The third difference between the two receptors is the position of the C-terminal  
16 activation domain. While the C-terminal activation domain forms  $\alpha$ -helices in both  
17 receptors, the domain in the rat TR- $\alpha$  LBD follows a proline-rich turn, and lies against the  
18 receptor to contribute part of the binding cavity. In contrast, the activation domain in the  
19 unliganded hRXR $\alpha$ , is part of a longer helix which projects into the solvent.

20 These differences lead to a model for an alternate conformation of the TR LBD  
21 assumed in the absence of ligand. In the unliganded TR, the subdomain of the receptor  
22 surrounding the hormone binding cavity is loosely packed, with the binding cavity occluded  
23 by a partly unstructured H11 providing a partial core for the receptor.

24 Upon binding hormone, residues which form a coil in the unbound receptor engage  
25 the ligand, and continues H11. The ordering of H11 could unblock the hydrophobic cavity,  
26 allowing H7 and H8 to interact with hormone. The extended hydrophobic cavity then  
27 collapses around the hormone, generating the compact bound structure.

28 It is possible to predict ligand-induced conformational changes in the C-terminal  
29 activation domain that rely, in part, on an extended structure in the unliganded TR that  
30 repacks upon ligand binding. The ligand-induced conformation change can be subtle since  
31 the amino acid sequence of the rat TR- $\alpha$  in the turn (393-PTELFPP-399) significantly

1 reduces the propensity of the peptide chain of the rat TR- $\alpha$  to form an  $\alpha$ -helix and therefore  
2 repacking can be accomplished with a minor change in volume.

3 After the ligand-induced conformational change occurs, it is likely that the  
4 conformation of the C-terminal activation domain in the bound structure changes packing  
5 compared to the unbound form of the receptor. Binding of the ligand improves the stability  
6 of the activation domain. The activation domain packs loosely even in the bound structure,  
7 as measured by the distribution of packing interactions for the entire LBD. The packing  
8 density for the activation domain, defined as the number of atoms within 4.5Å, is 1.5  
9 standard deviations below the mean. For comparison, another surface helix, H1, is 0.5  
10 standard deviations below the mean and the most poorly packed part of the structure, the  
11 irregular coil from residues Ile196-Asp206, is 2.0 standard deviations below the mean.  
12 Moreover, the majority of packing contacts for the C-terminal domain in the bound receptor  
13 are provided either by residues which interact with ligand, such as His381, or by the ligand  
14 itself. The conformation of these residues can be expected to be different in the bound and -  
15 unbound receptors, and by extension the conformation of C-terminal activation domain which  
16 relies upon these interactions. Without the stabilization provided by a bound ligand, it is  
17 likely that the C-terminal activation domain is disordered prior to hormone binding.

18 The interrelation of ligand-induced conformational changes is evident as described  
19 herein. For example, His381 from H11 and Phe405 from H12 interact in the bound  
20 structure to provide a specific hydrogen bond to the phenolic hydroxyl. The ligand-induced  
21 changes which affect H11 and H12 are reinforcing, and lead to the formation of the compact,  
22 bound state.

23 Comparison of the TR- $\alpha$  and TR- $\beta$  LBD structures shows similar packing of the  
24 helices when complexed with the ligand Triac.

25

## 26 COMPUTATIONAL METHODS USING THREE DIMENSIONAL MODELS AND EXTENSIONS OF 27 LIGANDS

28 The three-dimensional structure of the liganded TR receptor is unprecedented, and  
29 will greatly aid in the development of new nuclear receptor synthetic ligands, such as thyroid  
30 receptor antagonists and improved agonists, especially those that bind selectively to one of  
31 the two TR isoforms ( $\alpha$  or  $\beta$ ). In addition, this receptor superfamily is overall well suited to

1 modern methods including three-dimensional structure elucidation and combinatorial  
2 chemistry such as those disclosed in EP 335 628, U.S. patent 5,463,564, which are  
3 incorporated herein by reference. Structure determination using X-ray crystallography is  
4 possible because of the solubility properties of the receptors. Computer programs that use  
5 crystallography data when practicing the present invention will enable the rational design of  
6 ligand to these receptors. Programs such as RASMOL can be used with the atomic  
7 coordinates from crystals generated by practicing the invention or used to practice the  
8 invention by generating three dimensional models and/or determining the structures involved  
9 in ligand binding. Computer programs such as INSIGHT and GRASP allow for further  
10 manipulation and the ability to introduce new structures. In addition, high throughput  
11 binding and bioactivity assays can be devised using purified recombinant protein and modern  
12 reporter gene transcription assays described herein and known in the art in order to refine the  
13 activity of a CDL.

14 Generally the computational method of designing a nuclear receptor synthetic ligand -  
15 comprises two steps:

16 1) determining which amino acid or amino acids of a nuclear receptor LBD interacts  
17 with a first chemical moiety (at least one) of the ligand using a three dimensional model of a  
18 crystallized protein comprising a nuclear receptor LBD with a bound ligand, and

19 2) selecting a chemical modification (at least one) of the first chemical moiety to  
20 produce a second chemical moiety with a structure to either decrease or increase an  
21 interaction between the interacting amino acid and the second chemical moiety compared to  
22 the interaction between the interacting amino acid and the first chemical moiety.

23 As shown herein, interacting amino acids form contacts with the ligand and the center  
24 of the atoms of the interacting amino acids are usually 2 to 4 angstroms away from the center  
25 of the atoms of the ligand. Generally these distances are determined by computer as  
26 discussed herein and in McRee 1993, however distances can be determined manually once  
27 the three dimensional model is made. Examples of interacting amino acids are described in  
28 Appendix 2. See also Wagner *et al.*, *Nature* 378(6558):670-697 (1995) for stereochemical  
29 figures of three dimensional models. More commonly, the atoms of the ligand and the atoms  
30 of interacting amino acids are 3 to 4 angstroms apart. The invention can be practiced by  
31 repeating steps 1 and 2 to refine the fit of the ligand to the LBD and to determine a better



1 ligand, such as an agonist. As shown in the **FIGURES** the three dimensional model of TR  
2 can be represented in two dimensions to determine which amino acids contact the ligand and  
3 to select a position on the ligand for chemical modification and changing the interaction with  
4 a particular amino acid compared to that before chemical modification. Structural  
5 comparison of LBD isoforms complexed with the same or similar ligand permit identification  
6 of fiducial and adjustable amino acids that can be exploited in designing isoform-specific  
7 ligands through chemical modification. "Fiducial" refers to amino acids that form rigid  
8 features of the ligand binding cavity. "Adjustable" refers to amino acids that form less rigid  
9 features of the ligand binding cavity. The chemical modification may be made using a  
10 computer, manually using a two dimensional representation of the three dimensional model  
11 or by chemically synthesizing the ligand. The three dimensional model may be made using  
12 Appendix 2 and the **FIGURES**. As an additional step, the three dimensional model may be  
13 made using atomic coordinates of nuclear receptor LBDs from crystallized protein as known  
14 in the art, see McRee 1993 referenced herein.

15 The ligand can also interact with distant amino acids after chemical modification of  
16 the ligand to create a new ligand. Distant amino acids are generally not in contact with the  
17 ligand before chemical modification. A chemical modification can change the structure of  
18 the ligand to make as new ligand that interacts with a distant amino acid usually at least 4.5  
19 angstroms away from the ligand. Often distant amino acids will not line the surface of the  
20 binding cavity for the ligand, as they are too far away from the ligand to be part of a pocket  
21 or surface of the binding cavity.

22 The interaction between an atom of a LBD amino acid and an atom of an LBD ligand  
23 can be made by any force or attraction described in nature. Usually the interaction between  
24 the atom of the amino acid and the ligand will be the result of a hydrogen bonding  
25 interaction, charge interaction, hydrophobic interaction, van der waals interaction or dipole  
26 interaction. In the case of the hydrophobic interaction it is recognized that this is not a per  
27 se interaction between the amino acid and ligand, but rather the usual result, in part, of the  
28 repulsion of water or other hydrophilic group from a hydrophobic surface. Reduction or  
29 enhancement of the interaction of the LBD and a ligand can be measured by standard binding  
30 procedures, calculating or testing binding energies, computationally or using thermodynamic  
31 or kinetic methods as known in the art.



1 Chemical modifications will often enhance or reduce interactions of an atom of a LBD  
2 amino acid and an atom of an LBD ligand. Steric hinderance will be a common means of  
3 changing the interaction of the LBD binding cavity with the activation domain. Chemical  
4 modifications are preferably introduced at C-H, C- and C-OH position in ligands, where the  
5 carbon is part of the ligand structure which remains the same after modification is complete.  
6 In the case of C-H, C could have 1, 2 or 3 hydrogens, but usually only one hydrogen will be  
7 replaced. The H or OH are removed after modification is complete and replaced with the  
8 desired chemical moiety.

9 Because the thyroid receptor is a member of the larger superfamily of hormone-  
10 binding nuclear receptors, the rules for agonist and antagonist development will be  
11 recognized by one skilled in the art as useful in designing ligands to the entire superfamily.  
12 Examining the structures of known agonists and antagonists of the estrogen and androgen  
13 receptors supports the generality of antagonist mechanism of action as shown in FIG. 10.

14 The overall folding of the receptor based on a comparison of the reported structure of  
15 the unliganded RXR and with amino acid sequences of other superfamily members reveals  
16 that the overall folding of receptors of the superfamily is similar. Thus, it is predicted from  
17 the structure that there is a general pattern of folding of the nuclear receptor around the  
18 agonist or antagonist ligand.

19 The three dimensional structure of a nuclear receptor with a ligand bound leads to the  
20 nonobvious observation that a nuclear receptor folds around agonist ligands, as the binding  
21 cavity fits the agonist, especially the agonist's molecular recognition domain, and antagonists  
22 commonly have chemical structures that extend beyond the ligand, especially the agonist, and  
23 would prohibit folding of the receptor around the ligand to form a buried binding cavity or  
24 other groups that have the same effect. The location of the extension could affect the folding  
25 in various ways as indicated by the structure. Such extensions on antagonists are shown in  
26 FIG. 10 for various receptors and compared to the corresponding agonist.

27 For example, an extension towards the carboxy-terminal activation helix affects the  
28 packing/folding of this helix into the body of the receptor. This in turn can affect the ability  
29 of this portion of the nuclear receptor to interact with other proteins or other portions of the  
30 receptor, including transcriptional transactivation functions on the opposite end of the linear  
31 receptor, or the receptor's amino terminus that may interact directly or indirectly with the

1 carboxy-terminal transactivation domain (including helix 12). Extensions in this direction  
2 can also affect the packing of helix 11 of TR (or its analogous helix in nuclear receptors) into  
3 the body of the receptor and selectively affect dimerization and heterodimerization of  
4 receptors. An extension pointing towards helix 1 can affect the relationship of the DNA  
5 binding domain and hinge regions of the receptors with the ligand binding domain and  
6 selectively or in addition affect the receptors' binding to DNA and/or interactions of  
7 receptors with proteins that interact with this region of the receptor. Other extensions  
8 towards helix 11 can be made to affect the packing of this helix and helices 1 and 10 and  
9 thereby homo- and hetero-dimerization. Such chemical modifications can be assessed using  
10 the computational methods described herein. It is also possible that, in some cases,  
11 extensions may protrude through the receptor that is otherwise completely or incompletely  
12 folded around the ligand. Such protruding extensions could present a steric blockade to  
13 interactions with co-activators or other proteins.

14 The three dimensional structure with the ligand buried in the binding cavity  
15 immediately offers a simple description of a nuclear receptor that has a binding cavity that  
16 contains hinges and a lid, composed of one or more structural elements, that move to  
17 accommodate and surround the ligand. The ligand to TR can be modified on specific sites  
18 with specific classes of chemical groups that will serve to leave the lid and hinge region in  
19 open, partially open or closed states to achieve partial agonist or antagonist functions. In  
20 these states, the biological response of the TR is different and so the structure can be used to  
21 design particular compounds with desired effects.

22 Knowledge of the three-dimensional structure of the TR-T<sub>3</sub> complex leads to a general  
23 model for agonist and antagonist design. An important novel feature of the structural data is  
24 the fact that the T<sub>3</sub> ligand is completely buried within the central hydrophobic core of the  
25 protein. Other ligand-receptor complexes belonging to the nuclear receptor superfamily will  
26 have a similarly buried ligand binding site and therefore this model will be useful for  
27 agonist/antagonist design for the entire superfamily.

28 When design of an antagonist is desired, one needs either to preserve the important  
29 binding contacts of natural hormone agonist while incorporating an "extension group" that  
30 interferes with the normal operation of the ligand-receptor complex or to generate the  
31 requisite binding affinity through the interactions of the extensions with receptor domains.

1 The model applied to antagonist design and described herein is called the "Extension  
2 Model." Antagonist compounds for nuclear receptors should contain the same or similar  
3 groups that facilitate high-affinity binding to the receptor, and in addition, such compounds  
4 should contain a side chain which may be large and/or polar. This side chain could be an  
5 actual extension, giving it bulk, or it could be a side group with a charge function that differs  
6 from the agonist ligand. For example, substitution of a CH<sub>3</sub> for CH<sub>2</sub>OH at the 21-position,  
7 and alteration at the 11-position from an OH group to a keto group of cortisol generates  
8 glucocorticoid antagonist activity (Robsseau, G.G., *et. al.*, *J. Mol. Biol.* 67:99-115 (1972)).  
9 However, in most cases effective antagonists have more bulky extensions. Thus, the  
10 antiglucocorticoid (and antiprogestin) RU486 contains a bulky side group at the 11-position  
11 (Horwitz, K.B. *Endocrine Rev.* 13:146-163 (1992)). The antagonist compound will then  
12 bind within the buried ligand binding site of the receptor with reasonably high affinity (100  
13 nM), but the extension function will prevent the receptor-ligand complex from adopting the  
14 necessary conformation needed for transcription factor function. The antagonism (which  
15 could be in an agonist or antagonist) may manifest itself at the molecular level in a number  
16 of ways, including by preventing receptor homo/heterodimer formation at the HRE, by  
17 preventing coactivator binding to receptor monomers, homodimers or homo/heterodimers, or  
18 by a combination of these effects which otherwise prevent transcription of hormone  
19 responsive genes mediated by ligand-induced effects on the HRE. There are several  
20 antagonist compounds for nuclear receptors in the prior art (see also Horwitz, K.B.,  
21 *Endocrine Rev.* 13:146-163 (1992), Raunnaud J.P. *et. al.*, *J. Steroid Biochem.* 25:811-833  
22 (1986), Keiel S., *et. al.*, *Mol. Cell. Biol.* 14:287-298 (1994) whose antagonist function can  
23 be explained by the extension hypothesis. These compounds are shown in FIG. 10 along  
24 with their agonist counterparts. Each of these antagonists contains a large extension group  
25 attached to an agonist or agonist analogue core structure. Importantly, these antagonist  
26 compounds were discovered by chance and not designed with a structure-function hypothesis  
27 such as the extension principle.

28 One method of design of a thyroid antagonist using the extension hypothesis is  
29 provided below as a teaching example. The three-dimensional structure of the TR- $\alpha$  Dimit  
30 complex combined with structure-activity data published in the prior art, especially those  
31 reference herein, can be used to establish the following ligand-receptor interactions which are

1 most critical for high-affinity ligand binding. A physical picture of these interactions is  
2 shown in **FIG. 6**. The figure describes the isolated essential contacts for ligand binding.  
3 Because the ligand is buried in the center of the receptor, the structural spacing between  
4 these isolated interactions is also important. Thus, our present knowledge of this system  
5 dictates that, for this example, a newly designed ligand for the receptor must contain a  
6 thyronine structural skeleton, or two substituted aryl groups joined by a one-atom spacer.

7 The general structure for an antagonist designed by the extension hypothesis is  
8 exemplified in the following general description of the substituents of a TR antagonist  
9 (referring to Formula 1): R1 can have anionic groups such as a carboxylate, phosphonate,  
10 phosphate, sulfate or sulfite and is connected to the ring with a 0 to 3 atom linker,  
11 comprising one or more C, O, N, S atoms, and preferably a 2 carbon linker. Such R1 can  
12 be optionally substituted with an amine (e.g. -NH<sub>2</sub>). R3 and R5 are small hydrophobic  
13 groups such as -Br, -I, or -CH<sub>3</sub>. R3 and R5 can be the same substituents or different. R<sub>3</sub>'  
14 can be a hydrophobic group that may be larger than those of R3 and R5, such as -I, -CH<sub>3</sub>, -  
15 isopropyl, -phenyl, -benzyl, 5 and 6 ring heterocycles. R<sub>4</sub>' is a group that can participate in  
16 a hydrogen bond as either a donor or acceptor. Such groups include -OH, -NH<sub>2</sub>, and -SH.  
17 R<sub>5</sub>' is an important extension group that makes this compound an antagonist. R<sub>5</sub>' can be a  
18 long chain alkyl (e.g. 1 to 9 carbons, straight chain or branched), aryl (benzyl, phenyl and  
19 substituted benzyl and phenyl rings (e.g. with halogen, alkyl (1 and 5 carbons) and optionally  
20 connected to the ring by a -CH<sub>2</sub>-), heterocycle (e.g. 5 or 6 atoms, preferably 5 carbons and  
21 1 nitrogen, or five carbons), which can optionally include polar (e.g. -OH, -NH<sub>2</sub>, and -SH),  
22 cationic (e.g. -NH<sub>3</sub>, N(CH<sub>3</sub>)<sub>3</sub>), or anionic (carboxylate, phosphonate, phosphate or sulfate)  
23 groups. R<sub>5</sub>' can also be a polar (e.g. -OH, -NH<sub>2</sub>, and -SH), cationic (e.g. -NH<sub>3</sub>, -  
24 N(CH<sub>3</sub>)<sub>3</sub>), and anionic (carboxylate, phosphonate, phosphate or sulfate) groups. X is the  
25 spacer group that appropriately positions the two aromatic rings. This group is usually a  
26 one-atom spacer, such as O, S, SO, SO<sub>2</sub>, NH, NZ where Z is an alkyl, CH<sub>2</sub>, CHOH, CO,  
27 C(CH<sub>3</sub>)OH, and C(CH<sub>3</sub>)(CH<sub>3</sub>). X also may be NR<sub>7</sub>, CHR<sub>7</sub>, CR<sub>7</sub>, R<sub>7</sub>, where R<sub>7</sub> is an alkyl,  
28 aryl or 5- or 6-membered heterocyclic aromatic. R2, R6, R2' and R6' can be -F, and -Cl  
29 and are preferably H.

30 A TR ligand can also be described as a substituted phenylated 3,5 diiodo tyrosine with  
31 substituted R5' and R3' groups. R5' can be a long chain alkyl (e.g. 4 to 9 carbons, straight



1 chain or branched), aryl (benzyl, phenyl and substituted benzyl and phenyl rings (e.g. with  
2 halogen, alkyl (1 and 5 carbons) and optionally connected to the ring by a -CH<sub>2</sub>-),  
3 heterocycle (e.g. 5 or 6 atoms, preferably 5 carbons and 1 nitrogen, or five carbons), which  
4 can optionally include polar (e.g. -OH, -NH<sub>2</sub>, and -SH), cationic (e.g. -NH<sub>3</sub>, N(CH)<sub>3</sub>), or  
5 anionic (carboxylate, phosphonate, phosphate or sulfate) groups. R<sub>5</sub>' can also be a polar  
6 (e.g. -OH, -NH<sub>2</sub>, and -SH), cationic (e.g. -NH<sub>3</sub>, N(CH)<sub>3</sub>), and anionic (carboxylate,  
7 phosphonate, phosphate or sulfate) groups. R<sub>3</sub>' can be -IsoPr, halogen, -CH<sub>3</sub>, alkyl (1 to 6  
8 carbons) or aryl (benzyl, phenyl and substituted benzyl and phenyl rings (e.g. with halogen,  
9 alkyl (1 and 5 carbons) and optionally connected to the ring by a -CH<sub>2</sub>-), heterocycle (e.g. 5  
10 or 6 atoms, preferably 5 carbons and 1 nitrogen, or five carbons), which can optionally  
11 include polar (e.g. -OH, -NH<sub>2</sub>, and -SH), cationic (e.g. -NH<sub>3</sub>, N(CH)<sub>3</sub>), or anionic  
12 (carboxylate, phosphonate, phosphate or sulfate) groups.

13 A TR antagonist can also be a modified T<sub>3</sub> agonist (having a biphenyl structure)  
14 wherein R<sub>5</sub>' is alkyl, aryl, 5- or 6-membered heterocyclic aromatic, heteroalkyl, heteroaryl, -  
15 arylalkyl, heteroaryl alkyl, polyaromatic, polyheteroaromatic, polar or charged groups,  
16 wherein said R<sub>5</sub>' may be substituted with polar or charged groups. The R<sub>5</sub>' groups are  
17 defined, as described herein.

18 Using these methods the ligands of this example preferably have the following  
19 properties:

- 20 1. The compounds should bind to the TR with high affinity (for example 100 nM).
- 21 2. The compounds should bind the receptor in the same basic orientation as the
- 22 natural hormone.
- 23 3. The extension group R<sub>5</sub>' should project toward the activation helix (C-terminal
- 24 helix) of the receptor.
- 25 4. The appropriate substituent at R<sub>5</sub>' should perturb the activation helix from its
- 26 optimal local structure needed for mediating transcription.

27 Antagonists may also be designed with multiple extensions in order to block more  
28 than one aspect of the folding at any time.

29 TR ligands (e.g. super agonists) can be designed (and synthesized) to enhance the  
30 interaction of at least one amino acid with at least one chemical moiety on the ligand's  
31 molecular recognition domain. One method is to enhance the charge and polar interactions



1 by replacing the carboxylate of T<sub>3</sub> (R1 position) with phosphonate, phosphate, sulfate or  
2 sulfite. This enhances the interaction with Arg 262, Arg 266 and Arg 228. The interaction  
3 of at least one amino acid with at least one chemical moiety on the ligand's molecular  
4 recognition domain can also be enhanced by increasing the size of R1 group to fill the space  
5 occupied by water when Dimit is bound (referring to R1). Preferably the group has a  
6 complementary charge and hydrophobicity to the binding cavity.

7 Another way of improving the interaction of at least one amino acid with at least one  
8 chemical moiety on the ligand's molecular recognition domain is to restrict the conformation  
9 of the dihedral angle between the two phenyl rings of the thyronine ligand in solution. In  
10 solution the planes of two phenyl rings are orthogonal where the dihedral angle is 90°. In  
11 the TR Dimit structure, the dihedral angle is close to 60°. A TR ligand design that fixes the  
12 angle between the two phenyl rings will lead to tighter binding. Such a ligand may be made  
13 by connecting the R6' and the R5 positions of a thyronine or a substituted thyronine-like  
14 biphenyl. The size of the cyclic connection can fix the angle between the two phenyl rings.-  
15 Referring specifically to Formula 1, the following cyclic modifications are preferred: 1) R<sub>5</sub> is  
16 connected to R<sub>6</sub>', 2) R<sub>3</sub> is connected to R<sub>2</sub>' or 3) R<sub>5</sub> is connected to R<sub>6</sub>' and R<sub>3</sub> is connected  
17 to R<sub>2</sub>'. The connections can be made by an alkyl or heteroalkyl chain having between 1 to 6  
18 atoms and preferably from 2 to 4 carbon atoms or other atoms. Any position of the  
19 heteroalkyl chain can be N, O, P or S. The S and P heteroatoms along said heteroalkyl chain  
20 are in any of their possible oxidative states. The N heteroatom or any carbon along the alkyl  
21 or heteroalkyl chain may have one or more Z substituents, wherein Z is alkyl, heteroalkyl,  
22 aryl, heteroaryl, 5- or 6-membered heterocyclic aromatic. These compounds can be claimed  
23 with the proviso that Formula 1 does not include any prior art compound as of the priority  
24 filing date of this application.

25 The interaction of at least one amino acid with at least one chemical moiety on the  
26 ligand's molecular recognition domain can also be enhanced by selecting a chemical  
27 modification that fills the unfilled space between a TR ligand and the LBD in the area of the  
28 bridging oxygen (such as in T3, Triac or Dimit). Thus, a slighter larger moiety that replaces  
29 the ether oxygen can enhance binding. Such a linker may be a mono- or geminal-  
30 disubstituted carbon group. A group approximately the same size as oxygen but with greater

1 hydrophobicity is preferred as well as small, hydrophobic groups for the disubstituted  
2 carbon.

3 Compounds of Formula I or derivatives thereof that modulate TR activity also may be  
4 designed and selected to interact with a conformationally constrained structural feature of a  
5 TR LBD that is conserved among TR LBD isoforms to increase TR-specific selectivity.  
6 Conserved structural features of a TR LBD include residues found in equivalent positions of  
7 TR LBD isoforms which interact with a conserved structural feature of a compound  
8 comprising the biphenyl scaffold ( $\phi$ -X- $\phi$ ) or a single phenyl scaffold ( $\phi$ -X or X- $\phi$ ) of  
9 Formula I. Conformationally constrained structural features of a TR LBD include residues  
10 that have their natural flexible conformations fixed by various geometric and physical-  
11 chemical constraints, such as local backbone, local side chain, and topological constraints.  
12 These types of constraints are exploited to restrict positioning of atoms involved in receptor-  
13 ligand recognition and binding. For example, comparison of atomic models of TR LBD  
14 isoforms bound to thyronine and thyronine-like ligands reveal that certain residues which  
15 contact the ligands are restricted to particular topological shapes and angles of rotation about  
16 bonds. These include Met259, Leu276, Leu292, His381, Gly290, Ile221, and Phe401 of  
17 TR- $\alpha$ . The corresponding positions in TR- $\beta$  include Met313, Leu330, Leu346, His435,  
18 Gly344, Ile275 and Phe455, respectively.

19 Selectivity imparted by conformationally constrained features of both the receptor and  
20 compound are of particular interest. For example, compounds of Formula I comprising  
21 constrained cyclic carbons and substituent groups that interact with a constrained feature of a  
22 TR LBD can be exploited to further increase binding specificity while reducing the potential  
23 for cross-over interaction with other receptors. These include hydrophobic and/or  
24 hydrophilic contacts between constrained residues of a TR LBD and atomic groups of the  
25 following constituents of the compound in reference to Formula I: (i) the biphenyl rings; (ii)  
26 the R3-substituent; (iii) the R3'-substituent; and (iv) the R4'-substituent.

27 For example, contacts to the phenyl moiety comprising the R1, R2, R3, R5 and R6  
28 substituents, i.e., the ring proximal to the polar pocket (the "inner ring"), include a cycle  
29 carbon atom that interacts with an atom of a hydrophobic residue of a TR LBD, such as a  
30 carbon and oxygen atom of Met259 and a carbon atom of Leu276 of TR- $\alpha$ , or Met313 and  
31 Leu330 of TR- $\beta$ , where the cycle carbon is about 3.0 to 4.0Å from the atom of the

hydrophobic group. For example, comparison of TR- $\alpha$  complexed with T3 and TR- $\beta$  complexed with GC-1 reveals the following conserved inner ring contacts:

Ligand	TR LBD			
	TR- $\alpha$ Residue	Atom	Distance	
T3/Atom				
C11	Met259	C	3.95	
C11	Met259	O	3.59	
C11	Met259	CB	3.77	
C7	Leu276	CD2	3.80	
C9	Leu276	CD2	3.70	
GC1/Atom	TR- $\beta$ Residue	Atom	Distance	
C11	Met313	C	3.85	
C11	Met313	O	3.41	
C11	Met313	CB	3.79	
C7	Leu330	CD2	3.56	
C9	Leu330	CD2	3.63	

Contacts to the phenyl moiety comprising the R2', R3', R4', R5' and R6' substituents, i.e., the ring distal to the polar pocket (the "outer ring"), include a cyclic carbon atom that interacts with an atom of a hydrophobic residue of a TR LBD, such as a carbon atom of Leu292 of TR- $\alpha$ , or Leu346 of TR- $\beta$ , where the cyclic carbon atom is about 3.0 to 4.0A from the atom of the hydrophobic residue. For example, comparison of TR- $\alpha$  complexed with T3 and TR- $\beta$  complexed with GC-1 reveals the following conserved outer ring contacts:

Ligand	TR LBD			
	TR- $\alpha$ Residue	Atom	Distance	
T3/Atom				
C6	Leu292	CD2	3.58	
C8	Leu292	CD2	3.50	
GC1/Atom	TR- $\beta$ Residue	Atom	Distance	
C6	Leu346	CD2	3.77	
C8	Leu346	CD2	3.80	

Contacts to the R3-substituent include an atom that interacts with a carbon atom of a hydrophobic residue of a TR LBD, such as Ile221 of TR- $\alpha$ , or Ile275 of TR- $\beta$ , where the R3-substituent atom is about 3.0 to 4.0A from the carbon atom of the hydrophobic residue.

For example, comparison of TR- $\alpha$  complexed with T3 and TR- $\beta$  complexed with GC-1 reveals the following conserved R3-substituent contacts:

Ligand	TR LBD		
	TR- $\alpha$ Residue	Atom	Distance
T3/Atom	Ile221	CG1	4.01
I1			
GC1/Atom	TR- $\beta$ Residue	Atom	Distance
C19	Ile275	CG1	3.98

Contacts to the R3'-substituent include an atom that interacts with an atom of a hydrophobic or hydrophilic residue of a TR LBD, such as an oxygen atom of Gly290 of TR- $\alpha$ , or Gly344 of TR- $\beta$ , where the R3'-substituent atom is about 3.0 to 4.0A from the atom of the hydrophobic or hydrophilic residue. For example, comparison of TR- $\alpha$  complexed with T3 and TR- $\beta$  complexed with GC-1 reveals the following conserved R4'-substituent, phenolic hydroxyl contacts:

Ligand	TR LBD		
	TR- $\alpha$ Residue	Atom	Distance
T3/Atom	Gly290	O	3.50
I2			
GC1/Atom	TR- $\beta$ Residue	Atom	Distance
C18	Gly344	O	3.60

Contacts to the R4'-substituent comprising a phenolic hydroxyl include carbon and oxygen atoms that interact with a hydrophobic or hydrophilic residue of a TR LBD, such as a carbon and nitrogen atom of His381 of TR- $\alpha$ , or His435 of TR- $\beta$ , where the R4'-substituent atom is about 2.0 to 4.0A from an atom of the hydrophobic or hydrophilic residue. For example, comparison of TR- $\alpha$  complexed with T3 and TR- $\beta$  complexed with GC-1 reveals the following conserved R4'-substituent, phenolic hydroxyl contacts:

<u>Ligand</u>	<u>TR LBD</u>			
T3/Atom	TR- $\alpha$ Residue	Atom	Distance	
C10	His381	CD2	3.97	
O1	His381	CD2	3.39	
O1	His381	CE1	3.82	
C8	His381	NE2	3.47	
C10	His381	NE2	3.55	
O1	His381	NE2	2.70	

<u>GC1/Atom</u>	TR- $\beta$ Residue	Atom	Distance	
C10	His435	CD2	3.89	
O1	His435	CD2	3.64	
O1	His435	CE1	3.79	
C8	His435	NE2	3.44	
C10	His435	NE2	3.33	
O1	His435	NE2	2.77	

Contacts to the R4'-substituent also may include an atom that interacts with a carbon atom of a hydrophobic residue of a TR LBD, such as Phe401 of TR- $\alpha$ , or Phe455 of TR- $\beta$ , for defining agonist activity, i.e., proper presentation of helix-12 (H12) of the TR LBD following ligand binding. The R4'-substituent atom is about 3.0 to 4.0A from the carbon atom of the hydrophobic group. For example, comparison of TR- $\alpha$  complexed with T3 and TR- $\beta$  complexed with GC-1 reveals the following conserved R4'-substituent contacts:

<u>Ligand</u>	<u>TR LBD</u>			
T3/Atom	TR- $\alpha$ Residue	Atom	Distance	
O1	Phe401	CE1	3.52	
O1	Phe401	CZ	3.32	
GC1/Atom	TR- $\beta$ Residue	Atom	Distance	
O1	Phe455	CE1	3.40	
O1	Phe455	CZ	3.22	

Comparison of atomic models of TR LBD isoforms complexed with the same and/or different ligands therefore facilitates the identification of new compounds that fit spacially and preferentially into a TR LBD. Modeling, comparison of TR-ligand overlays, and comparison of TR LBD isoforms also permit identification of conformationally conserved structural features of TR LBD/ligand contacts. Exploiting conformational constraints of the LBD-ligand interaction identified by such methods therefore improves the design and



1 identification of new compounds having increased selectivity for binding a particular type of  
2 nuclear receptor, such as TR.

#### 3 4 **TR- $\alpha$ AND TR- $\beta$ SELECTIVITY FOR THE THYROID HORMONE RECEPTOR**

5 Using the method described herein ligands can be designed that selectively bind to the  
6 alpha more than the beta TR or vice versa. The X-ray crystallographic structure of the rat  
7 TR- $\alpha$  LBD provides insight into design of such ligands.

8 The three dimensional structure reveals that the major difference between the TR- $\alpha$   
9 and TR- $\beta$  in the ligand binding cavity resides in amino acid Ser 277 (with the side group  
10 -CH<sub>2</sub>OH) in the rat TR- $\alpha$  and whose corresponding residue is 331, asparagine (with the side  
11 group -CH<sub>2</sub>CONH<sub>2</sub>), in the human TR- $\beta$ . The side chain in human TR- $\beta$  is larger, charged  
12 and has a different hydrogen bonding potential, which would allow the synthesis of  
13 compounds that discriminate between this difference. The Ser277 (Asn331 in TR- $\beta$ ) forms  
14 part of the polar pocket of the TR LBD, indicating that for TR- $\alpha$  versus TR- $\beta$   
15 discrimination, ligands can be designed to contain chemical modification of the R1-  
16 substituent with reference to Formula I that exploit this difference.

17 For example, in the complex of TR- $\alpha$  with Triac, Ser277 does not participate in  
18 ligand binding. The absence of a role for Ser277 (Asn331 in beta) is consistent with the  
19 equal affinity of Triac for the alpha and beta isoforms, and indirectly supports the contention  
20 that alpha/beta selectivity resides in the amino acid substitution Ser277 to Asn331 and its  
21 interaction with Arg228. The effect of the amino acid substitution is further evident when  
22 the interactions of Asn331 and Arg282 in the structures of the TR- $\beta$  LBD complexed with  
23 GC-1 or Triac are compared with those of Ser277 and Arg228 in the TR- $\alpha$  LBD. In the  
24 complex with GC-1, Asn331 forms a hydrogen bond to Arg282, which in turn forms a  
25 hydrogen bond with the carboxylate of GC-1, a pattern that resembles the interactions of  
26 Ser277 and Arg228 in the complexes of the TR- $\alpha$  LBD complexed with T<sub>3</sub> or Triac.  
27 However, in the complex of TR- $\beta$  with Triac, Arg282 rotates away from Asn331 and the  
28 ligand, instead forming hydrogen bonds to residues Thr287 and Asp291 of H3. Therefore,  
29 differences exist between the two isoforms in the conformation of the polar pocket,  
30 depending on the nature of the ligand R1-substituent, indicating that certain substituents may  
31 interact preferentially with the conformation of a given isoform.

1 Comparing overlays of various ligands bound to the TR- $\alpha$  versus TR- $\beta$  LBDs shows  
2 the positioning of the ligand to be very similar. Surprisingly, comparison of the volume and  
3 area for the TR- $\alpha$  and TR- $\beta$  LBDs bound by the same or different ligands unexpectedly  
4 shows that the cubic space or volume available for accommodating ligand binding by the TR-  
5  $\beta$  LBD ( $645 \pm 28.28 \text{ \AA}^3$ ) is larger and more flexible than that of the TR- $\alpha$  LBD ( $596.25 \pm$   
6  $7.97 \text{ \AA}^3$ ) (Table 1). The volume of the ligand binding cavity for TR- $\alpha$  varies over a narrow  
7 range of about 8+, with a maximum difference of about 16+. In contrast, the volume of  
8 the ligand binding cavity for TR- $\beta$  differs by nearly 40+ between the complexes with GC-1  
9 and Triac. There also is a difference in the volume of the ligand binding cavity when  
10 comparing the same ligand bound to TR- $\alpha$  and TR- $\beta$ . For example, TR- $\alpha$  and TR- $\beta$   
11 complexed with Triac differ in LBD volume by about  $36 \text{ \AA}^3$ . Comparison of TR- $\alpha$  and TR-  
12  $\beta$  bound to Dimit and GC-1, respectively, which ligands have similar volume/area and  
13 superpositioned architecture, show that the difference in LBD volume is about  $75 \text{ \AA}^3$ . These  
14 differences are attributed primarily to variable movement and interaction of side chain groups  
15 with ligand substituents of the phenyl moiety ( $\phi$ ) of the biphenyl scaffold ( $\phi$ -X- $\phi$ ) located  
16 proximal to the polar pocket, e.g., R1-substituents in reference to Formula I. In contrast,  
17 the volume available in the hydrophobic pocket for both the TR- $\alpha$  and TR- $\beta$  LBDs is  
18 substantially the same. For example, binding of Triac to the TR- $\beta$  LBD displaces the side  
19 chain of Arg 282 providing approximately  $60 \text{ \AA}^3$  in the polar pocket cavity, exposing the  
20 polar pocket to bulk solvent exchange. For GC1 bound to the TR- $\beta$  LBD, approximately  $14$   
21  $\text{ \AA}^3$  is due to side chain motion of Met310, and approximately  $44 \text{ \AA}^3$  is due to side chain  
22 motion of Arg320, the combination of which increases the size of the polar pocket in the TR-  
23  $\beta$  LBD. This extra pliability also may explain the absence of ordered water in the polar  
24 pocket of TR- $\beta$  LBD bound to Triac or GC-1, which is in contrast to the ordered water  
25 found in the polar pocket of TR- $\alpha$  LBD bound to Dimit, IpBr2 or T3.

Table 1*				
rTR- $\alpha$				
	<u>Dimit</u>	<u>Triac</u>	<u>IpBr2</u>	<u>T3</u>
TR LBD (volÅ <sup>3</sup> /areaÅ <sup>2</sup> )	590/456	589/440	601/474	605/472
Ligand (volÅ <sup>3</sup> /areaÅ <sup>2</sup> )	303/314	333/326	326/330	355/346
Complementarity	0.65	0.68	0.66	0.71
hTR- $\beta$				
	<u>GC-1</u>	<u>Triac</u>		
TR LBD (volÅ <sup>3</sup> /areaÅ <sup>2</sup> )	665/575	625/474		
Ligand (volÅ <sup>3</sup> /areaÅ <sup>2</sup> )	294/310	333/326		
Complementarity	0.61	0.67		

\*TR LBD volume and area are reported in Angstroms measured by GRASP. Complementarity is determined as defined in Lawrence *et al.*, *J. Mol. Biol.* 234:946-950 (1993).

Residue Ser277 in TR- $\alpha$  and the corresponding residue Asn331 of TR- $\beta$  also contribute to the volumetric differences observed in the polar pockets of these two TR isoforms. And substitution of the Asn331 of hTR- $\beta$  with serine has the affect of modifying ligand binding affinity of TR- $\beta$  so that it resembles that of TR- $\alpha$  (See Example 5). Taken together, differences in hydrogen bonding of atoms of the side chain group of Ser277 in TR- $\alpha$  and Asp331 in TR- $\beta$  extending from the equivalent backbone position in these TR LBDs and the more restricted polar pocket of the TR- $\alpha$  LBD further supports the concept of designing TR LBD isoform-specific ligands having substituents that fit spacially and preferentially into the polar pocket of either the TR- $\alpha$  or TR- $\beta$  LBDs. Exploitation of this difference provides an additional means for computational design of isoform-specific TR agonists and antagonists.

In terms of ligand design, these differences mean that for  $\beta$ -selective ligands, some or all of the following differences should be exploited:

1. The presence of a larger side chain asparagine.
2. The ability of the carbonyl group on the side chain to provide a strong hydrogen bond acceptor.
3. The ability of the amido group on the side chain to provide a two hydrogen bond donors.
4. Adjustment of polarity to reorganize the trapped water in the T3 pocket.

1           5.       Greater size and flexibility of the polar pocket.

2           In terms of pharmaceutical design, these differences mean that for  $\alpha$ -selective ligands,  
3 some or all of the following differences should be exploited:

4           1.       The presence of a smaller side group.

5           2.       The ability of the hydroxyl on the  $-\text{CH}_2\text{OH}$  side group carbonyl group on the  
6 side chain to provide a weak hydrogen donor.

7           3.       Adjustment of polarity to reorganize the trapped water in the T3 pocket.

8           4.       Smaller size and limited flexibility of the polar pocket.

9           In both cases these differences can be exploited in a number of ways. For example,  
10 they can also be used with a software set for construction of novel organic molecules such as  
11 LUDI from Biosym-MSI. An example of designing TR- $\beta$  selective ligands is increasing the  
12 polarity of a ligand substituent located in the polar pocket of a TR LBD through addition of  
13 one or more ligand groups having a formal negative charge and/or negative dipole charge  
14 that interacts with a formal positive charge and/or positive dipole charge of a group in the  
15 polar pocket of the LBD. This exploits preferential interactions, such as with the additional  
16 positive charge contributed by Asn 331 in TR- $\beta$ . Another example of a TR- $\beta$  selective  
17 ligand is one that comprises one or more groups which fit spacially into the TR- $\beta$  LBD polar  
18 pocket. This exploits spacial differences between TR LBD isoforms, such as the larger and  
19 more flexible polar pocket of TR- $\beta$ .

## 21 METHODS OF TREATMENT

22           The compounds of Formula 1 can be useful in medical treatments and exhibit  
23 biological activity which can be demonstrated in the following tests:

24           (i)       the induction of mitochondrial  $\alpha$ -glycerophosphate dehydrogenase (GPDH:EC  
25 1.1.99.5). This assay is particularly useful since in certain species e.g. rats it is induced  
26 specifically by thyroid hormones and thyromimetics in a close-related manner in responsive  
27 tissues e.g. liver, kidney and the heart (Westerfield, W.W., Richert, D.A. and Ruegamer,  
28 W.R., *Endocrinology* (1965) 77:802). The assay allows direct measurement in rates of a  
29 thyroid hormone-like effect of compounds and in particular allows measurement of the direct  
30 thyroid hormone-like effect on the heart. Other measurements included parameters such as

1 heart rate and cardiac enzymes including  $\text{Ca}^{++}$  ATPase,  $\text{Na}^{++}/\text{K}^{+}$  ATPase, myosin isoforms  
2 and specific liver enzymes;

3 (ii) the elevation of basal metabolic rate as measured by the increase in whole  
4 body oxygen consumption (see e.g., Barker *et al.*, *Ann. N. Y. Acad. Sci.*, (1960) 86:545-  
5 562);

6 (iii) the stimulation of the rate of beating of atria isolated from animals previously  
7 dosed with thyromimetics (see e.g., Stephan *et al.*, *Biochem. Pharmacol.* (1992) 13:1969-  
8 1974; Yokoyama *et al.*, *J. Med. Chem.*, (1995) 38:695-707);

9 (iv) the change in total plasma cholesterol levels as determined using a cholesterol  
10 oxidase kit (for example, the Merck CHOD iodine colorimetric kit. see also, Stephan *et al.*  
11 (1992));

12 (v) the measurement of LDL (low density lipoprotein) and HDL (high density  
13 lipoprotein) cholesterol in lipoprotein fractions separated by ultracentrifugation; and p (vi) the  
14 change in total plasma triglyceride levels as determined using enzymatic color tests, for  
15 example the Merck System GPO-PAP method.

16 The compounds of Formula 1 can be found to exhibit selective thyromimetic activity  
17 in these tests,

18 (a) by increasing the metabolic rate of test animals, and raising hepatic GPDH  
19 levels at doses which do not significantly modify cardiac GPDH levels.

20 (b) by lowering plasma cholesterol and triglyceride levels, and the ratio of LDL to  
21 HDL cholesterol at doses which do not significantly modify cardiac GPDH levels.

22 The compounds of Formula 1 may therefore be used in therapy, in the treatment of  
23 conditions which can be alleviated by compounds which selectively mimic the effects of  
24 thyroid hormones in certain tissues whilst having little or no direct thyromimetic effect on the  
25 heart. For example, compounds of Formula 1 which raise hepatic GPDH levels and  
26 metabolic rate at doses which do not significantly modify cardiac GPDH levels are indicated  
27 in the treatment of obesity.

28 Agonists of Formula 1 will lower total plasma cholesterol, the ratio of LDL-  
29 cholesterol to HDL-cholesterol and triglyceride levels at doses which do not significantly  
30 modify cardiac GPDH levels are indicated for use as general antihyperlipidaemic  
31 (antihyperlipoproteinaemic) agents i.e. in the treatment of patients having elevated plasma



1 lipid (cholesterol and triglyceride) levels. In addition, in view of this effect on plasma  
2 cholesterol and triglyceride, they are also indicated for use as specific anti-  
3 hypercholesterolemic and anti-hypertriglyceridaemic agents.

4 Patients having elevated plasma lipid levels are considered at risk of developing  
5 coronary heart disease or other manifestations of atherosclerosis as a result of their high  
6 plasma cholesterol and/or triglyceride concentrations. Further, since LDL-cholesterol is  
7 believed to be the lipoprotein which induces atherosclerosis, and HDL-cholesterol believed to  
8 transport cholesterol from blood vessel walls to the liver and to prevent the build up of  
9 atherosclerotic plaque, anti-hyperlipidemic agents which lower the ratio of LDL-cholesterol  
10 to HDL cholesterol are indicated as anti-atherosclerotic agents, herein incorporated by  
11 reference U.S. patents 4,826,876 and 5,466,861.

12 The present invention also provides a method of producing selective thyromimetic  
13 activity in certain tissues except the heart which comprises administering to an animal in  
14 need thereof an effective amount to produce said activity of a compound of Formula 1 or a -  
15 pharmaceutically acceptable salt thereof.

16 The present invention also relates to a method of lowering plasma lipid levels and a  
17 method of lowering the ratio of LDL-cholesterol to HDL-cholesterol levels by suitably  
18 administering a compound of this invention or a pharmaceutically acceptable salt thereof.

19 In addition, compounds of Formula 1 may be indicated in thyroid hormone  
20 replacement therapy in patients with compromised cardiac function.

21 In therapeutic use the compounds of the present invention are usually administered in  
22 a standard pharmaceutical composition.

23 The present invention therefore provides in a further aspect pharmaceutical  
24 compositions comprising a compound of Formula 1 or a pharmaceutically acceptable salt  
25 thereof and a pharmaceutically acceptable carrier. Such compositions include those suitable  
26 for oral, parenteral or rectal administration.

## 27 28 PHARMACEUTICAL COMPOSITIONS

29 Compounds of Formula 1 and their pharmaceutically acceptable salts which are active  
30 when given orally can be formulated as liquids for example syrups, suspensions or  
31 emulsions, tablets, capsules and lozenges.

1 A liquid composition will generally consist of a suspension or solution of the  
2 compound or pharmaceutically acceptable salt in a suitable liquid carrier(s), for example  
3 ethanol, glycerine, sorbitol, non-aqueous solvent such as polyethylene glycol, oils or water,  
4 with a suspending agent, preservative, surfactant, wetting agent, flavoring or coloring agent.  
5 Alternatively, a liquid formulation can be prepared from a reconstitutable powder.

6 For example a powder containing active compound, suspending agent, sucrose and a  
7 sweetener can be reconstituted with water to form a suspension; and a syrup can be prepared  
8 from a powder containing active ingredient, sucrose and a sweetener.

9 A composition in the form of a tablet can be prepared using any suitable  
10 pharmaceutical carrier(s) routinely used for preparing solid compositions. Examples of such  
11 carriers include magnesium stearate, starch, lactose, sucrose, microcrystalline cellulose and  
12 binders, for example polyvinylpyrrolidone. The tablet can also be provided with a color film  
13 coating, or color included as part of the carrier(s). In addition, active compound can be  
14 formulated in a controlled release dosage form as a tablet comprising a hydrophilic or  
15 hydrophobic matrix.

16 A composition in the form of a capsule can be prepared using routine encapsulation  
17 procedures, for example by incorporation of active compound and excipients into a hard  
18 gelatin capsule. Alternatively, a semi-solid matrix of active compound and high molecular  
19 weight polyethylene glycol can be prepared and filled into a hard gelatin capsule; or a  
20 solution of active compound in polyethylene glycol or a suspension in edible oil, for example  
21 liquid paraffin or fractionated coconut oil can be prepared and filled into a soft gelatin  
22 capsule. Compound of Formula 1 and their pharmaceutically acceptable salts which are  
23 active when given parenterally can be formulated for intramuscular or intravenous  
24 administration.

25 A typical composition for intra-muscular administration will consist of a suspension or  
26 solution of active ingredient in an oil, for example arachis oil or sesame oil. A typical  
27 composition for intravenous administration will consist of a sterile isotonic aqueous solution  
28 containing, for example active ingredient, dextrose, sodium chloride, a co-solvent, for  
29 example polyethylene glycol and, optionally, a chelating agent, for example ethylenediamine  
30 tetracetic acid and an anti-oxidant, for example, sodium metabisulphite. Alternatively, the

1 solution can be freeze dried and then reconstituted with a suitable solvent just prior to  
2 administration.

3 Compounds of structure (1) and their pharmaceutically acceptable salts which are  
4 active on rectal administration can be formulated as suppositories. A typical suppository  
5 formulation will generally consist of active ingredient with a binding and/or lubricating agent  
6 such as a gelatin or cocoa butter or other low melting vegetable or synthetic wax or fat.

7 Compounds of Formula 1 and their pharmaceutically acceptable salts which are active  
8 on topical administration can be formulated as transdermal compositions. Such compositions  
9 include, for example, a backing, active compound reservoir, a control membrane, liner and  
10 contact adhesive.

11 The typical daily dose of a compound of Formula 1 varies according to individual  
12 needs, the condition to be treated and with the route of administration. Suitable doses are in  
13 the general range of from 0.001 to 10 mg/kg bodyweight of the recipient per day.

14 Within this general dosage range, doses can be chosen at which the compounds of  
15 Formula 1 lower plasma cholesterol levels and raise metabolic rate with little or no direct  
16 effect on the heart. In general, but not exclusively, such doses will be in the range of from  
17 lower doses (0.001 to 0.5 mg/kg) to higher doses (0.5 to 10 mg/kg).

18 In addition, within the general dose range, doses can be chosen at which the  
19 compounds of Formula 1 lower plasma cholesterol levels and have little or no effect on the  
20 heart without raising metabolic rate. In general, but not exclusively, such doses will be in  
21 the range of from 0.001 to 0.5 mg/kg.

22 It is to be understood that the 2 sub ranges noted above are not mutually exclusive  
23 and that the particular activity encountered at a particular dose will depend on the nature of  
24 the compound of Formula 1 used.

25 Preferably, the compound of Formula 1 is in unit dosage form, for example, a tablet  
26 or a capsule so that the patient may self-administer a single dose. In general, unit doses  
27 contain in the range of from 0.05-100 mg of a compound of Formula 1. Preferred unit doses  
28 contain from 0.05 to 10 mg of a compound of Formula 1.

29 The active ingredient may be administered from 1 to 6 times a day. Thus daily doses  
30 are in general in the range of from 0.05 to 600 mg per day. Preferably, daily doses are in  
31 the range of from 0.05 to 100 mg per day. Most preferably from 0.05 to 5 mg per day.

## EXAMPLES

### EXAMPLE 1 - SYNTHESIS OF TR LIGANDS

Many TR ligands are known in the art, including T4 (thyroxine), T3, T2 and TS-9. See Jorgensen, Thyroid Hormones and Analogs, in 6 *Hormonal Proteins and Peptides, Thyroid Hormones* 107-204 (Choh Hao Li ed., 1978), incorporated by reference herein.

The syntheses of several TR ligands are described below.

#### Synthesis of TS1, TS2, TS3, TS4, TS5

TS1, TS2, TS3, TS4 and TS5 and analogs thereof can all be prepared by simple acylation of the nitrogen atom of any thyronine analog, including T3 (3,5,3'-triiodo-L-thyronine), T4 (thyroxine) and 3,5-diiodothyronine. TS1 and TS2 are synthesized by reacting T3 with  $\text{Ph}_2\text{CHCO}_2\text{NHS}$  (N-hydroxy succinimide-2,2-diphenylacetate) and  $\text{C}_{16}\text{H}_{33}\text{CO}_2\text{NHS}$ , respectively. TS3 is synthesized by reacting T3 with Fmoc-Cl (fluorenylmethyloxycarbonylchloride). TS4 is synthesized by reacting T3 with  $\text{tBOC}_2\text{O}$  (tBOC anhydride or di-t-butyldicarbonate). TS5, which differs from TS1-4 by having a -H instead of an -I at the  $\text{R}^1_3$  position, is synthesized by reacting 3,5-diiodothyronine with  $\text{tBOC}_2\text{O}$ . The general reaction scheme for TS1, TS2, TS3, TS4 and TS5 is depicted in FIG. 11. It should be noted that in the reaction scheme, both TS5 and its precursor both have a hydrogen rather than an iodine at the  $\text{R}^1_3$  position.

#### Synthesis of TS6 and TS7

TS6 is synthesized by reacting TS5 with paranitrophenylisocyanate. TS7 is synthesized by reacting TS6 with TFA (trifluoroacetic acid), which cleaves the tBOC group. These reactions are simple organic synthesis reactions that can be performed by anyone of ordinary skill in the art. The synthetic scheme for TS6 and TS7 is diagrammed in FIG. 12.

#### Synthesis of TS8

TS8 is synthesized by reacting TS5 with  $\text{Ph}_2\text{CHNH}_2$  (diphenylmethylaniline) in the presence of triethylamine and any amide forming condensing reagent, such as TBTU (hydroxybenztriazoleuronium tetrafluoroborate) or HBTU (hydroxybenztriazoleuronium hexafluorophosphate). The synthesis scheme for TS8 is depicted in FIG. 13.

## 1 SYNTHESIS OF 3,5-DIIODO-3'-ISOPROPYLTHYRONINE DERIVATIVES

2 For designing a class of antagonists, it is important to have a hydrophobic group at  
3 the 3' position as well as an extension at the 5' position. Preferred hydrophobic groups at  
4 the 3' position include: methyl, benzyl, phenyl, iodo, and heterocyclic structures. The  
5 synthesis of a 3,5-diiodo-3'-isopropyl-5'-substituted thyronine is described below. The  
6 example provided describes the specific steps for synthesizing the TS10 compound, but this  
7 general reaction scheme can be used by one of ordinary skill in the art to synthesize any  
8 number of 3,5,-diiodo-3'-isopropyl-5'-substituted thyronine derivatives, which are  
9 characterized by having an extension at the 5' position. Additional compounds of this class  
10 can be synthesized using known organic synthesis techniques.

11 The synthesis of TS10 is described below and is depicted in FIG. 14. Numbers used  
12 in the reaction scheme for TS10 indicating the reaction product for each step are in  
13 parentheses.

14 2-Formyl-6-isopropylanisole (1): 2-formyl-6-isopropylanisole (10.0 g, 61 mmol), as -  
15 made by Casiraghi, *et al.* JCS Perkin I, 1862 (1980) (incorporated by reference), is added  
16 dropwise to a suspension of sodium hydride (3.7 g, 153 mmol) in 50 mL THF and 50 mL of  
17 DMF in a round bottom flask. The addition generates an exothermic reaction and formation  
18 of a gray solid. Methyl iodide (26.0 g, 183 mmol) is then added dropwise and the reaction  
19 mixture is stirred at room temperature for 5 hours. The reaction mixture is quenched with  
20 20 mL of water, then poured into 500 mL of water, and is extracted with ether (2 x 300  
21 mL). The ether layers are combined, washed with water (5 x 1000 mL), dried over  
22 magnesium sulfate and concentrated in vacuo to provide 10.2 g (94%) of the title compound,  
23 with the following <sup>1</sup>H NMR (CDCl<sub>3</sub>) properties: δ 10.30 (s, 1H), 7.63 (d, 1H, J=3 Hz),  
24 7.50 (d, 1H, J=3 Hz), 7.13 (t, 1H, J=3 Hz), 3.81 (s, 3H), 3.31 (heptet, 1H, J=7.5 Hz),  
25 1.19 (d, 6H, J=7.5 Hz).

26  
27 2-(2-Hydroxynonyl)-6-isopropylanisole (not shown in scheme): Octylmagnesium  
28 chloride (8.4 mL, 16.9 mmol, 2.0 M) is added dropwise to a solution of 1 (1.5 g, 8.4 mmol)  
29 in 10 mL THF at -78°C. The reaction mixture is stirred for 2 hours with warming to room  
30 temperature. The reaction mixture is diluted with 50 mL ether and poured into 50 mL  
31 water. The ether layer is washed with brine (1 x 50 mL), dried over sodium sulfate, and



1 concentrated in vacuo. Flash chromatography (silica gel, 10% ether/hexane → 15%  
2 ether/hexane) provides 734 mg (30%) of the title compound with the following <sup>1</sup>H NMR  
3 (CDCl<sub>3</sub>) properties: δ 7.33-7.10 (m, 3H), 5.00 (br. s, 1H), 3.81 (s, 3H), 3.33 (heptet, 1H,  
4 J=7 Hz) 1.90-1.19 (m, 14H), 0.86 (t, 3H, J=6.5 Hz); HRMS (EI), found: 292.2404;  
5 calc'd: 292.2402.

6 2-nonyl-6-isopropylanisole (2): Compound 2 (663 mg, 2.3 mmol) is dissolved in  
7 solution of 5 mL ethanol and 5 mL acetic acid, and a spatula tip of palladium on carbon  
8 catalyst is added. The reaction mixture is then charged with hydrogen gas (using a simple  
9 balloon and needle) and the mixture is stirred at room temperature overnight. The next day,  
10 the reaction mixture is poured into ether (100 mL) and the ether layer is extracted with  
11 saturated sodium bicarbonate (3 x 100 mL). The ether layer is dried over sodium sulfate and  
12 concentrated *in vacuo* to provide 581 mg (91%) of (2) with the following <sup>1</sup>H NMR (CDCl<sub>3</sub>)  
13 properties: δ 7.14-7.00 (m, 3H), 3.75 (s, 3H), 3.36 (heptet, 1H, J=6.8 Hz), 2.63 (t, 2H,  
14 J=7.5 Hz), 1.68-1.15 (m, 14H), 0.86 (t, 3H, J=5.5 Hz); HRMS (EI), mass found:  
15 276.2459; calculated: 276.2453.

16 Thyronine adduct (4): Fuming nitric acid (0.071 mL) is added to 0.184 mL acetic  
17 anhydride chilled to -5°C. Iodine (66 mg) is added to this mixture followed by  
18 trifluoroacetic acid (0.124 mL). This mixture is stirred for 1 hour with warming to room  
19 temperature, at which point all of the iodine is dissolved. The reaction mixture was then  
20 concentrated *in vacuo* to provide an oily semi-solid material. The residue was dissolved in  
21 0.7 mL of acetic anhydride and cooled to -20°C. A solution of anisole (2) (581 mg, 2.1  
22 mmol) in 1.2 mL acetic anhydride and 0.58 mL TFA is added dropwise. The reaction  
23 mixture is stirred at -20° for 1 hour, then stirred overnight with warming to room  
24 temperature. The reaction mixture is partitioned between water and methylene chloride.  
25 The methylene chloride layer is dried over sodium sulfate and concentrated *in vacuo* to  
26 provide the iodonium salt (3) as an oil. This material is not purified or characterized, and is  
27 directly introduced into the coupling reaction.

28 N-Trifluoroacetyl-3,5-diiodotyrosine methyl ester (552 mg, 1.0 mmol) prepared  
29 according to the procedure of N. Lewis and P. Wallbank, *Synthesis* 1103 (1987)  
30 (incorporated by reference) and all of the crude iodonium salt (3) from above is dissolved in  
31 5 mL of anhydrous methanol. Diazabicyclo[5.4.0]undecane (DBU) (183 mg, 1.2 mmol) and

1 a spatula tip of copper-bronze are added and the resulting mixture is stirred at room  
2 temperature overnight. The next day, the reaction mixture is filtered, and the filtrate is  
3 concentrated *in vacuo*. The crude residue is purified by flash chromatography (silica gel,  
4 10% ethyl acetate/hexane) to provide 30 mg (4%) of the protected thyronine adduct (4).

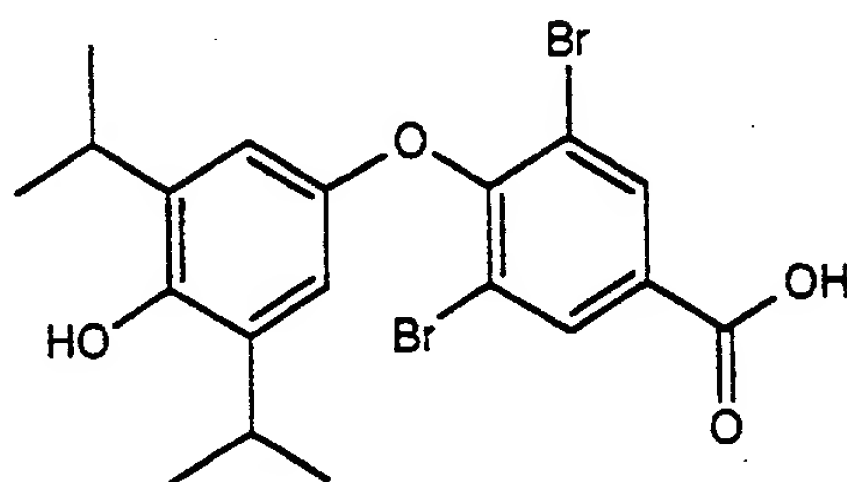
5 Deprotected thyronine (TS10): The protected thyronine 4 (30 mg, 0.04 mmol) is  
6 dissolved in a mixture of 2.25 mL acetic acid and 2.25 mL 49% hydrobromic acid. The  
7 reaction mixture is heated to reflux for 5 hours. The reaction mixture is cooled to room  
8 temperature, and the solvents are removed *in vacuo*. Water is added to triturate the oily  
9 residue into a gray solid. This solid material is filtered, washed with water, and dried over  
10  $P_2O_5$  *in vacuo* to provide 24 mg (81%) of the title compound, TS10, with the following  $^1H$   
11 NMR ( $CDCl_3$ ) properties:  $\delta$  7.57 (s, 1H), 6.86 (s, 1H), 6.45 (s, 1H), 6.34 (s, 1H), 4.81  
12 (m, 1H), 3.86 (s, 3H), 3.71 (s, 3H), 3.33-3.05 (m, 3H), 2.58-2.47 (m, 2H), 1.62-0.76 (m,  
13 23H); MS (LSIMS):  $M^+ = 817.0$ .

14 As mentioned above, this reaction scheme can be modified by one of ordinary skill in  
15 the art to synthesize a class of compounds characterized by 3,5-diiodo-3'-isopropylthyronine  
16 derivatives, wherein (1) the 3' isopropyl group can be replaced with a hydrophobic group,  
17 including methyl, benzyl, phenyl, iodo, and heterocyclic structures, and (2) a wide variety of  
18 chemical structures can be incorporated at the 5' position, including alkyl groups, planar  
19 aryl, heterocyclic groups, or polar and/or charged groups.

20 The aldehyde (1) in the above reaction scheme is a versatile synthetic intermediate  
21 which allows for the attachment of a variety of chemical moieties to the 5' position of the  
22 final thyronine derivative. In addition, a variety of chemical reactions can be used to attach  
23 the chemical moieties. These reactions are well known in the art and include organometallic  
24 additions to the aldehyde (including Grignard reagents, organolithiums, etc.), reductive  
25 amination reactions of the aldehyde with a primary or secondary amine, and Wittig  
26 olefination reactions with a phosphorous ylid or stabilized phosphonate anion. Other  
27 possibilities include reduction of the aldehyde to a benzyl alcohol allowing for etherification  
28 reactions at the 5' position. As mentioned above, these methods allow for a wide variety of  
29 chemical structures to be incorporated at the 5' position of the final thyronine derivative,  
30 including alkyl groups, planar aryl, heterocyclic groups or polar and/or charged groups.

31

1 Synthesis of 3, 5-dibromo-4-(3',5'-diisopropyl-4'-hydroxyphenoxy) benzoic acid  
2 (Compound 11).



3  
4  
5  
6  
7  
8 (a) A mixture of 2,6-diisopropyl phenol (20 g, 0.11 mol), potassium carbonate (62 g,  
9 0.45 mol), acetone (160 ml) and methyl iodide (28 ml, 0.45 mole) is refluxed for three days.  
10 The reaction mixture is filtered through celite, evaporated, dissolved in ether, washed twice  
11 with 1M sodium hydroxide, dried over magnesium sulphate and concentrated to afford 15.1 g  
12 (0.08 mol, 70%) of 2,6-diisopropyl anisole as a slightly yellow oil.

13 (b) Fuming nitric acid (12.4 ml, 265 mmol) is added dropwise to 31.4 ml of acetic  
14 anhydride which is cooled in a dry ice/carbon tetrachloride bath. Iodine 11.3 g, 44.4 mmol)  
15 is added in one portion followed by dropwise addition of trifluoroacetic acid (20.5 ml, 266  
16 mmole). The reaction mixture is stirred at room temperature until all the iodine is dissolved.  
17 Nitrogen oxides are removed by flushing nitrogen into the vessel. The reaction mixture is  
18 concentrated, the residue is dissolved in 126 ml of acetic anhydride and is cooled in a dry  
19 ice/carbon tetrachloride bath. To the stirred solution 2,6-diisopropylanisole (51 g, 266  
20 mmol) in 150 ml of acetic anhydride and 22.6 ml of trifluoroacetic acid is added dropwise.  
21 The reaction mixture is left to stand at room temperature over night and then is concentrated.  
22 The residue is taken up in 150 ml of methanol and treated with 150 ml of 10% aqueous  
23 sodium bisulfite solution and 1 liter of 2M sodium borotetrafluoride solution. After the  
24 precipitate aggregates, petroleum ether is added and the supernatant is decanted. The  
25 precipitate is triturated with petroleum ether, filtered, washed with petroleum ether and dried  
26 at room temperature in vacuo. This affords 34 g (57 mmol, 65%) of bis(3,5-diisopropyl-4-  
27 methoxyphenyl)iodonium tetrafluoroborate as a white solid.

28 (c) To a stirred solution of 3,5-dibromo-4-hydroxybenzoic acid (12 g, 40.5 mmol) in  
29 250 ml of methanol, thionyl chloride (3 ml) is added dropwise. The reaction mixture is  
30 refluxed for five days, water is added and the precipitated product is filtered off. The  
31 residue is dissolved in ethyl acetate. From the aqueous phase, methanol is removed by

1 concentration. The aqueous phase is then saturated with sodium chloride, and extracted with  
2 ethyl acetate. The combined organic phases are dried over magnesium sulphate, filtered and  
3 concentrated. This gives 12.5 g (40.5 mmol, 100%) of 3,5-dibromo-4-hydroxymethyl  
4 benzoate as a white crystalline solid.

5 (d) The products obtained in steps b and c are reacted with each other according to  
6 the following protocol. To bis(3,5-diisopropyl-4-methoxyphenyl)iodonium tetrafluoroborate  
7 (2.86 g, 4.8 mmole) and copper bronze (0.42 g, 6.4 mmole) in 7 ml. of dichloromethane at  
8 0°C is added dropwise a solution of 3,5-dibromo-4-hydroxymethyl benzoate (1.0 g, 3.2  
9 mmole) and triethylamine (0.36 g, 3.5 mmole) in 5 ml of dichloromethane. The reaction  
10 mixture is stirred in the dark for eight days and then is filtered through celite. The filtrate is  
11 concentrated and the residue is purified by column chromatography (silica gel, 97:3  
12 petroleum ether/ethyl acetate) to give 0.62 g (1.2 mmole, 39%) of 3,5-dibromo-4-(3',5'-  
13 diisopropyl-4'-methoxyphenoxy)methyl benzoate as a solid.

14 (e) The product from step d (0.2 g, 0.4 mmole) is dissolved in 2 ml.  
15 dichloromethane, is put under nitrogen and is cooled at -40°C. To the stirred solution is  
16 added 1M BBr<sub>3</sub> (1.2 ml, 1.2 mmole) dropwise. The reaction mixture is allowed to reach  
17 room temperature and then is left over night. It is cooled to 0°C and then hydrolyzed with  
18 water. Dichloromethane is removed by concentration and the aqueous phase is extracted  
19 with ethyl acetate. The organic phase is washed with 1M hydrochloric acid and brine. Then  
20 it is dried over magnesium sulphate, filtered and concentrated. The residue is  
21 chromatographed (silica, 96:3.6:0.4 dichloromethane/methanol/acetic acid) producing 93 mg  
22 (0.2 mmole, 51%) of 3,5-dibromo-4-(3',5'-diisopropyl-4'-hydroxyphenoxy)benzoic acid as a  
23 white solid. <sup>1</sup>H nmr (CDCl<sub>3</sub>) δ 1.23 (d, 12H, methyl), 3.11 (m, 2H, CH), 6.50 (s, 2H, 2,6-  
24 H) 8.33 (s, 2H, 2',6'-H).

25 Synthesis of addition ligands are described in U.S. Serial No. 08/877,792, filed June  
26 18, 1997 which is herein incorporated in its entirety by reference.

27 **TABLE 2** and **FIG. 15** depict the structures of several TR ligands in reference to  
28 Formula I.

TABLE 2

Cmpd	R <sub>3</sub>	R <sub>4</sub>	R <sub>5</sub>	R <sub>3</sub>	R <sub>4</sub>	R <sub>5</sub>	R <sub>1</sub>
*T <sub>4</sub>	-I	-O-	-I	-I	-OH	-H	-CH <sub>2</sub> CH(NH <sub>2</sub> )CO <sub>2</sub> H
*T <sub>4</sub>	-I	-O-	-I	-I	-OH	-I	-CH <sub>2</sub> CH(NH <sub>2</sub> )CO <sub>2</sub> H
TS1	-I	-O-	-I	-I	-OH	-H	-CH <sub>2</sub> CH[NHCOCH <sub>2</sub> ] <sub>2</sub> CO <sub>2</sub> H
TS2	-I	-O-	-I	-I	-OH	-H	-CH <sub>2</sub> CH[NHCO(CH <sub>2</sub> ) <sub>15</sub> CH <sub>3</sub> ]CO <sub>2</sub> H
TS3	-I	-O-	-I	-I	-OH	-H	-CH <sub>2</sub> CH[NH-FMOC]CO <sub>2</sub> H
TS4	-I	-O-	-I	-I	-OH	-H	-CH <sub>2</sub> CH[NH-tBOC]CO <sub>2</sub> H
TS5	-I	-O-	-I	-H	-OH	-H	-CH <sub>2</sub> CH[NH-tBOC]CO <sub>2</sub> H
TS6	-I	-O-	-I	-H	-OC(O)NH=Ø <sub>p</sub> NO <sub>2</sub>	-H	-CH <sub>2</sub> CH[NH-tBOC]CO <sub>2</sub> H
TS7	-I	-O-	-I	-I	-OC(O)NH=NHØNO <sub>2</sub>	-H	-CH <sub>2</sub> CH(NH <sub>2</sub> )CO <sub>2</sub> H
TS8	-I	-O-	-I	-H	-NH-CHØØ	-H	-CH <sub>2</sub> CH[NH-tBOC]CO <sub>2</sub> H
TS9	-I	-O-	-I	-IsoPr	-OH	-H	-CH <sub>2</sub> CH(NH <sub>2</sub> )CO <sub>2</sub> H
TS10	-I	-O-	-I	-IsoPr	-OH	-(CH) <sub>8</sub> - CH <sub>3</sub>	-CH <sub>2</sub> CH(NH <sub>2</sub> )CO <sub>2</sub> H

\* Prior Art Compound

-Ø: phenyl

-Ø<sub>p</sub>NO<sub>2</sub>: para nitro phenyl

## EXAMPLE 2 - RECEPTOR BINDING ASSAYS OF TR LIGANDS

To test the ability of synthesized TR ligands to bind to a thyroid receptor (TR), the binding affinity of a TR ligand for TR is assayed using TR's prepared from rat liver nuclei and <sup>125</sup>I T<sub>3</sub> as described in J.D. Apriletti, J.B. Baxter, and T.N. Lavin, *J. Biol. Chem.*, 263: 9409-9417 (1988). The apparent K<sub>d</sub>'s are calculated using the method described by Apriletti (1995) and Apriletti (1988). The apparent K<sub>d</sub>'s are presented in TABLE 3. The apparent K<sub>d</sub>'s (App.K<sub>d</sub>) are determined in the presence of the sample to be assayed, 1 nM [<sup>125</sup>I]T<sub>3</sub>, and 50µg/ml core histones, in buffer E (400 mM KCl, 200 mM potassium phosphate, pH 8.0, 0.5 mM EDTA, 1 mM MgCl<sub>2</sub>, 10% glycerol, 1 mM DTT) in a volume of 0.21 ml.



1 After incubation overnight at 4°C, 0.2 ml of the incubation mixture is loaded onto a Quick-  
 2 Sep Sephadex G-25 column (2.7 x 0.9 cm, 1.7 ml bed volume) equilibrated with buffer E.  
 3 The excluded peak of protein-bound [<sup>125</sup>I]T<sub>3</sub> is eluted with 1 ml of buffer E, collected in a  
 4 test tube, and counted. Specific T<sub>3</sub> binding is calculated by subtracting nonspecific binding  
 5 from total binding.

6 **TABLE 3**

7	Compound	App.Kd(nM)	Coactivation Assay RIP-140	EC <sub>50</sub> (M)
8	T <sub>3</sub>	0.06	+	10 <sup>-10</sup>
9	T <sub>4</sub>	2	+	10 <sup>-9</sup>
10	TS1	4	+	10 <sup>-7</sup>
11	TS2	1400	nd	nd
12	TS3	4	+	10 <sup>-8</sup>
13	TS4	8	+	nd
14	TS5	220	+	10 <sup>-6</sup>
15	TS6	>10000	nd	nd
16	TS7	260	+	10 <sup>-7</sup>
17	TS8	6000	nd	nd
18	TS9	1	+	10 <sup>-10</sup>
19	TS10	400	+	10 <sup>-6</sup>

20  
 21 +: RIP-140 Binding

22 -: RIP-140 Binding

23 nd: Not Determined

### 1 EXAMPLE 3 - INCREASED NUCLEAR PROTEIN COACTIVATION BY TR LIGANDS

2 To test the ability of TR ligands to activate the binding of TR to the nuclear activation  
3 protein RIP-140 (a nuclear protein that can bind to nuclear receptors, such as the estrogen  
4 receptor), a TR ligand is liganded to TR and then incubated with RIP-140 as described in V.  
5 Cavailles, *et al.*, *EMBO J.*, 14(15):3741- 3751 (1995), which is incorporated by reference  
6 herein. In this assay, 35<sub>s</sub>-RIP-140 protein binds to liganded TR but not unliganded TR.  
7 Many TR 35<sub>s</sub> ligands can activate RIP-140 binding as shown in TABLE 3.

### 9 EXAMPLE 4 - TR LIGAND BINDING AND TR ACTIVATION IN CULTURED CELLS

10 To test TR activation of transcription in a cellular environment, TR ligands are  
11 assayed for their ability to activate a reporter gene, chloramphenicol transferase ("CAT"),  
12 which has a TR DNA binding sequence operatively linked to it. Either GC or L937 cells  
13 (available from the ATCC) can be used, respectively). In such assays, a TR ligand crosses  
14 the cell membrane, binds to the TR, and activates the TR, which in turn activates gene  
15 transcription of the CAT by binding the TR DNA binding region upstream of the CAT gene.  
16 The effective concentration for half maximal gene activation (EC<sub>50</sub>) is determined by assaying  
17 CAT gene activation at various concentrations as described herein and in the literature. The  
18 results of CAT gene activation experiments are shown in TABLE 3.

### 20 CAT GENE ACTIVATION ASSAYS

21 Functional response to thyroid hormone (3,5,3'-triiodo-L-thyronine, T<sub>3</sub>) and TR  
22 ligands is assessed either in a rat pituitary cell line, GC cells, that contain endogenous  
23 thyroid hormone receptors (TRs) or U937 cells that contain exogenous TRs expressed as  
24 known in the art. GC cells are grown in 10-cm dishes in RPMI 1640 with 10% newborn  
25 bovine serum, 2 mM glutamine, 50 units/ml penicillin and 50 µg/ml streptomycin. For  
26 transfections, cells are trypsinized, resuspended in buffer (PBS, 0.1% glucose) and mixed  
27 with a TREtkCAT plasmid (10 mg) or phage in 0.5 ml buffer (15±5 million cells) and  
28 electroporated using a Bio-Rad gene pulser at 0.33 kvolts and 960 mF. The TREtkCAT  
29 plasmid contains two copies of a T<sub>3</sub> response element (AGGTCAcaggAGGTCA) cloned in  
30 the Hind III site of the pUC19 polylinker immediately upstream of a minimal (-32/+45)  
31 thymidine kinase promoter linked to CAT (tkCAT) coding sequences. After electroporation,

cells are pooled in growth medium (RPMI with 10% charcoal-treated, hormone stripped, newborn bovine serum), plated in 6-well dishes and treated with either ethanol or hormone. CAT activity is determined 24 hours later as described D. C. Leitman, R. C. J. Ribeiro, E. R. Mackow, J. D. Baxter, B. L. West, *J. Biol. Chem.* 266, 9343 (1991), which is incorporated by reference herein.

#### EFFECT OF TS-10 ON THE TRANSCRIPTIONAL REGULATION OF THE DR4-ALP REPORTER GENE IN THE PRESENCE OR ABSENCE OF T3.

**Characteristics of the TRAF cells:** TRAFa1 are CHO K1 cells stably transformed with an expression vector encoding the human thyroid hormone receptor  $\alpha$  1 and a DR4,ALP reporter vector; TRAFb1 are CHO K1 cells stably transformed with an expression vector encoding the human thyroid hormone receptor  $\beta$ 1 and a DR4-ALP reporter vector.

#### Interpretation of the effect of compound TS-10 on the transcriptional regulation of the DR4-ALP reporter gene in the presence or absence of T3.

**TRAFa1 reporter cells:** TS-10 alone (open circles) induces a partial activation of the expression of the ALP reporter protein amounting to approximately 27% of the maximal effect by the natural thyroid hormone T3. In the presence of T3 (filled circles), TS-10 has a weak antagonistic effect. The EC50 concentration for the agonistic effect of TS-10 and the EC50 concentration for its T3 antagonistic effect, respectively, is indicated in FIG. 18.

In FIG. 18, open and filled circles with dotted lines show the dose-dependent effect of TS-10/T3 on the toxicity marker (MTS/PMS), reduction of tetrazolium salt in the mitochondria, displayed on the right y-axis as optical density. There is no obvious toxic effect of TS-10 on the MTS-PMS marker but there is a clear effect on the morphology of the cells, as can be seen under the light microscope, at the highest concentration of TS-10 (32 mM) both in the absence and presence of T3, respectively (not shown in the figure).

1 **TRAFb1 reporter cells:** TS-10 alone (open circles) induces a partial activation of the  
2 expression of the ALP reporter protein amounting to approximately 35% of the maximal  
3 effect by T3. The EC50 concentration for the agonistic effect of TS-10 is indicated in FIG.  
4 19. In the presence of T3 (filled circles), TS-10 shows, if anything, a slight potentiation of  
5 the T3 effect on the expression of the ALP reporter protein. The T3 inhibitory effect of TS-  
6 10 at its highest concentration used (32 mM) is a toxic effect rather than T3 antagonism.

7  
8 In FIG. 19, open and filled circles with dotted lines show the dose-dependent effect of TS-  
9 10/T3 on the toxicity marker (MTS/PMS), reduction of tetrazolium salt in the mitochondria,  
10 displayed on the right y-axis as optical density. There is no obvious toxic effect of TS-10 on  
11 the MTS-PMS marker but a clear effect on the morphology of the cells can be observed,  
12 under the light microscope, at the highest concentration of TS-10 (32 mM) both in the  
13 absence and presence of T3, respectively (not shown in the figure).

14  
15 **HepG2 (HAF18) reporter cells:** TS-10 alone (open circles) induces a partial activation of  
16 the expression of the ALP reporter protein amounting to slightly more than 50% of the  
17 maximal effect by T3. The EC50 concentration for the agonistic effect of TS-10 is indicated  
18 in FIG. 20. In the presence of T3 (filled circles), TS-10 shows no effect i.e. no T3  
19 antagonism nor potentiation/additive effect to T3. Open and filled circles with dotted lines  
20 show the dose-dependent effect of TS-10/T3 on the toxicity marker (MTS/PMS), reduction  
21 of tetrazolium salt in the mitochondria, displayed on the right y-axis as optical density.  
22 There is no obvious toxic effect of TS-10 on the MTS/PMS marker or on the morphology of  
23 the cells, as can be observed using a light microscope, at any concentration of TS-10/T3  
24 used.

## 25 26 **Example 5 - Comparisons of Human TR- $\alpha$ and Human TR- $\beta$**

### 27 **Competition for [ $^{125}$ I]T<sub>3</sub> binding to TR LBD by T<sub>3</sub> and Triac**

28 The drug, Triac, is a thyroid hormone agonist. Triac is 3,5,3'-triiodothyroacetic acid  
29 and is described in Jorgensen, Thyroid Hormones and Analogs in 6 *Hormonal Proteins and*  
30 *Peptides, Thyroid Hormones* at 150-151 (1978). Another compound that can be used in place  
31 of Triac is 3,5-diiodo-3'-isopropylthyroacetic acid. Competition assays are performed to

1 compare the displacement of [ $^{125}$ I]T<sub>3</sub> from binding with human TR- $\alpha$  LBD or human TR- $\beta$   
2 LBD by unlabeled T<sub>3</sub> or Triac. The results of such assays are depicted in FIG. 16.

3 Standard binding reactions are prepared containing 1 nM [ $^{125}$ I]T<sub>3</sub>, 30 fmol of human  
4 TR- $\alpha$  (empty symbols) or  $\beta$  (solid symbols), and various concentrations of competing  
5 unlabeled T<sub>3</sub> (circles) or Triac (triangles). Assays are performed in duplicate.

#### 7 Competition for [ $^{125}$ I]T<sub>3</sub> binding to variant TR LBD by T<sub>3</sub>, Triac and GC-1

8 The following assays residues involved in selective binding among TR isoforms.

9 Competition assays are performed to compare the displacement of [ $^{125}$ I]T<sub>3</sub> from binding with  
10 wild-type human TR- $\alpha$  LBD or human TR- $\beta$  LBD, to a variant form of the TR LBDs by  
11 unlabeled T<sub>3</sub>, Triac or GC-1. A variant TR- $\alpha$  or TR- $\beta$  is constructed by substituting an  
12 amino acid found in the corresponding position of the other TR isoform. For example,  
13 asparagine 331 in human TR- $\beta$  corresponds to serine 277 in human TR- $\alpha$ . To test binding  
14 specificity contributed by this position, a variant human TR- $\beta$  is constructed that contains  
15 asparagine 331 substituted with a serine residue (designated Asn331Ser or N331S). Binding  
16 assays are described in *Apriletti et al.* (Protein Expression and Purification 6:363-370  
17 (1995)). The results of such assays are depicted in FIG. 27, and summarized in Table 4  
18 below.

20 TABLE 4

21 Effect of TR- $\beta$  Substitution N331S on Binding Affinity

Ligand	Native TR- $\alpha$	Native TR- $\beta$	Mutant TR- $\beta$
T3	20 pM	60 pM	100 pM
T4	600	3000	ND
Triac	20	20	100
IpBr <sub>2</sub>	17	ND	ND
Dimit	6000	8000	ND
GC-1	200	40	400



Competition curves comparing wildtype TR- $\beta$  versus the variant TR- $\beta$  N331S for binding T3, Triac or GC-1 show that the affinity of the mutant receptor for Triac was reduced to approximately the same as for T3 (vs. 3-fold greater in wild type) so that the relative affinities are similar to wild-type TR- $\alpha$ . The affinity for GC-1 was also reduced to several fold less than T3, as is seen with TR- $\alpha$ .

Comparison of the affinity of TR- $\beta$  variant N331S to the native TRs for selected ligands is as follows:

Native TR- $\alpha$  for various ligands (T3, T4, Triac, IpBr2, Dimit, GC-1):

IpBr<sub>2</sub> > Triac = T3 > GC-1 > T4 > Dimit

Native TR- $\beta$  (T3, T4, Triac, Dimit, GC-1)

Triac > GC-1  $\geq$  T3 > T4 > Dimit

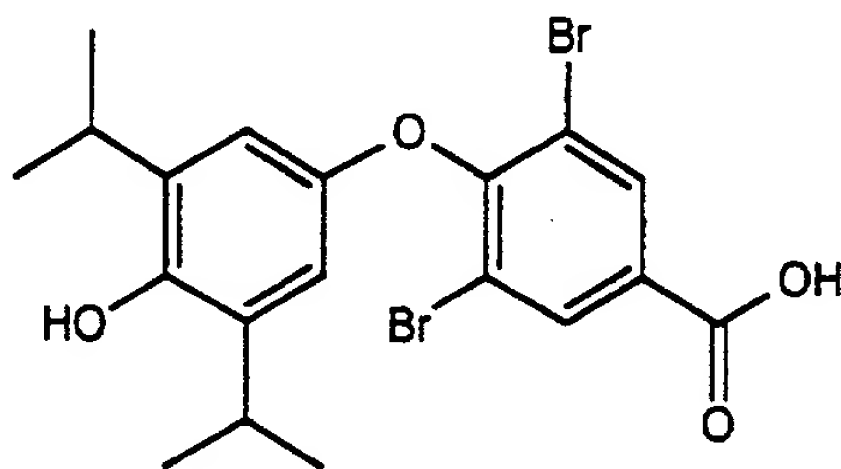
Variant TR- $\beta$  (N331S) (T3, Triac, GC-1)

Triac = T3 > GC-1.

### Scatchard Analysis of [<sup>125</sup>I]T<sub>3</sub> Binding to TR

Human TR- $\alpha$  (left panel) or human TR- $\beta$  (right panel) is assayed for T<sub>3</sub> binding in the presence of increasing concentrations of [<sup>125</sup>I]T<sub>3</sub>. The apparent equilibrium dissociation constant (20 pM for  $\alpha$  and 67 pM for  $\beta$ ) is calculated by linear regression analysis and is depicted in FIG. 17.

**3, 5-DIBROMO-4-(3',5'-DIISOPROPYL-4'-HYDROXYPHENOXY) BENZOIC ACID IS A TR- $\alpha$  SELECTIVE SYNTHETIC LIGAND.**



3, 5-dibromo-4-(3',5'-diisopropyl-4'-hydroxyphenoxy) benzoic acid (Compound 11), the structure of which is drawn above, is assayed for binding to the two different isoforms of the TR, TR- $\alpha$  and TR- $\beta$ . Compound 11 exhibits an IC<sub>50</sub> of 1.6  $\mu$ M for binding to TR- $\alpha$

1 and an IC<sub>50</sub> of 0.91  $\mu$ M for binding to TR- $\beta$ . Assays for determining selective binding to  
2 the TR- $\alpha$  or TR- $\beta$  LBD can include reporter assays, as described herein. See also  
3 Hollenberg, *et al.*, *J. Biol. Chem.*, (1995) 270(24):14274-14280.

#### 4 5 **EXAMPLE 6 - PREPARATION AND PURIFICATION OF A TR- $\alpha$ LBD**

6 Rat TR- $\alpha$  LBD, residues Met122 - Val410, is purified from *E. coli* ("LBD-122/410").

7 The expression vector encoding the rat TR- $\alpha$  LBD is freshly transfected into *E. coli* strain  
8 BL21(DE3) and grown at 22°C in a 50-liter fermenter using 2x LB medium. At an A<sub>600</sub> of  
9 2.5-3, IPTG is added to 0.5 mM and growth is continued for 3 h before harvesting. The  
10 bacterial pellet is quickly frozen in liquid nitrogen and stored at -70°C until processed.

11 Extraction and purification steps are carried out at 4°C. The bacteria are thawed in  
12 extraction buffer (20MM Hepes, pH 8.-, 1 mM EDTA, 0.1% MTG, 0.1 mM PMSF, and  
13 10% glycerol) at a ratio of 10 ml buffer/g bacteria. Bacteria are lysed by incubation for 15  
14 min. with 0.2 mg/ml lysozyme and sonicated at maximum power while simultaneously  
15 homogenized with a Brinkmann homogenizer (Model PT 10/35 with generator PTA 35/2)  
16 until the solution loses its viscosity. After centrifugation for 10 min at 10,000 g, the  
17 supernatant is adjusted to 0.4 M KCl, treated with 0.6% PEI to precipitate fragmented DNA,  
18 and centrifuged for 10 min at 10,000 g. The rat TR- $\alpha$  LBD in the supernatant is then  
19 precipitated with 50% ammonium sulfate and centrifuged for 10 min at 10,000 g. The  
20 precipitate is resuspended with buffer B (20 mM Hepes, pH 8.0, 1 mM EDTA, 1 mM DTT,  
21 0.1 mM PMSF, 0.01% Lubrol, and 10% glycerol) to a final conductivity of 9 mS/cm  
22 (approx. 0.7 M ammonium sulfate) and centrifuged 1 h at 100,000g. The supernatant is  
23 frozen in liquid nitrogen and stored at -70°C.

24 The crude extract is thawed, bound with a tracer amount of [<sup>125</sup>I]T<sub>3</sub>, and loaded  
25 directly onto a phenyl-Toyopearl hydrophobic interaction column (2.6 x 18 cm, 95 ml bed  
26 volume) at 1.5 ml/min. The column is eluted with a 2-h gradient from 0.7 ammonium  
27 sulfate, no glycerol to no salt, 20% glycerol in buffer C (20 mM Hepes, pH 8.0, 0.5 mM  
28 EDTA, 1 mM DTT, 0.2 mM PMSF). The rat TR- $\alpha$  LBD prebound to tracer [<sup>125</sup>I]T<sub>3</sub> (less  
29 than 0.005% of total rat TR- $\alpha$  LBD) is detected using a flow-through gamma emission  
30 detector, whereas unliganded rat TR- $\alpha$  LBD is assayed by postcolumn [<sup>125</sup>I]T<sub>3</sub> binding assays  
31 (described herein).

1 The phenyl-Toyopearl unliganded rat TR- $\alpha$  LBD peak fractions are pooled, diluted  
2 with buffer B to a conductivity of 0.5 mS/cm (equivalent to approx. 20 mM ammonium  
3 sulfate), loaded onto a TSK-DEAE anion-exchange column (2 x 15 cm, 47 ml bed volume) at  
4 4 ml/min, and eluted with a 60-min gradient from 50 to 200 mM NaCl in buffer B.

5 The unliganded rat TR- $\alpha$  LBD peak fractions from TSK-DEAE are pooled, diluted  
6 twofold with buffer B, loaded at 0.75 ml/min on a TSK-heparin HPLC column (0.8 x 7.5  
7 cm, 3 ml bed volume), and eluted with a 50 to 400 mM NaCl gradient in buffer B.

8 The pool of unliganded rat TR- $\alpha$  LBD peak fractions from the TSK-heparin column is  
9 adjusted to 0.7 M ammonium sulfate, loaded at 0.75 ml/min on a TSK-phenyl HPLC column  
10 (0.8 x 7.5 cm, 3 ml bed volume), and eluted with a 60-min gradient from 0.7 M ammonium  
11 sulfate without glycerol to no salt with 20% glycerol in buffer C. The fractions containing  
12 unliganded rat TR- $\alpha$  LBD are pooled and incubated with a five fold excess of hormone for 1  
13 h, the salt concentration is adjusted to 0.7 M ammonium sulfate, and the sample is reloaded  
14 and chromatographed on the same column as described above.

#### 15 16 **EXAMPLE 7 - CRYSTALLIZATION OF LIGANDED TR- $\alpha$ LBD**

17 Material from a single LBD-122/410 preparation is divided into batches, and  
18 quantitatively bound with one of the following ligands: Dimit, T<sub>3</sub>, or Triac IpBr<sub>2</sub>  
19 (3,5dibromo-3'-isopropylthyronine) for the final purification step.

20 To maintain full saturation of rat TR- $\alpha$  LBD with a ligand, and to prepare the  
21 complex for crystallization, the ligand-bound rat TR- $\alpha$  LBD is concentrated and desalted in  
22 an Amicon Centricon-10 microconcentrator (McGrath et al, *Biotechniques*, (1989) 7:246-247,  
23 incorporated by reference herein), using 10 mM Hepes (pH 7.0), 3.0 mM DTT, and 1.0 nM  
24 to 10 nM ligand.

25 Factorial crystallization screening trials (Jancarik & Kim, *J. Appl. Crystallogr.* (1991)  
26 24:409-411, incorporated by reference herein) are carried out for rat TR- $\alpha$  LBD bound to  
27 selected ligands using hanging-drop vapor diffusion at 17°C (with 1  $\mu$ l protein solution, 1  $\mu$ l  
28 precipitant solution and a 0.5 ml reservoir using silanized coverslip: (McPherson, *Preparation*  
29 *and Analysis of Protein Crystals* (1982), incorporated by reference herein). Rat TR- $\alpha$  LBD  
30 is not stable at 4°C and is stored at -80°C, where it maintains its avidity for hormone and its  
31 crystallizability for approximately two to three months. These procedures are carried out as

1 described in McGrath, M.E. *et al.*, *J. Mol. Biol.* (1994) 237:236-239 (incorporated by  
2 reference). Crystals are obtained in condition 21 of the screening trials (Jancarik & Kim  
3 1991) and conditions are then optimized. Wedge-shaped crystals are reproducibly obtained  
4 with hanging-drop vapor fusion at 22°C with 15% 2-methyl-2,4-pentanediol (MPD), 0.2 M  
5 ammonium acetate and 0.1 M sodium cacodylate (pH 6.7), 3 mM DTT, with 2  $\mu$ l protein  
6 solution, 1  $\mu$ l precipitant solution and a 0.6 ml reservoir using silanized coverslip, and with  
7 8.7 mg/ml (Dimit), 5.5 mg/ml (IpBr<sub>2</sub>), 5 mg/ml (Triac), or 2.3 mg/ml (T<sub>3</sub>) over a period of  
8 three days. Under these conditions, diffraction quality crystals (dimension 0.5 x 0.2 x  
9 0.0075 mm<sup>3</sup>) can be grown at ambient temperature (22°C). The best crystals have a limiting  
10 dimension of approximately 100  $\mu$ m and are obtained at a protein concentration between 2.3  
11 and 8.7 mg/ml in the presence of 3 mM DTT. The crystals are of the monoclinic space  
12 group C2, with one monomer in the asymmetric unit.

#### 13 14 **EXAMPLE 8 - CRYSTALLIZATION OF HUMAN TR- $\beta$ LBD COMPLEXED WITH T<sub>3</sub>, TRIAC,** 15 **OR GC-1**

16 Human TR- $\beta$  LBD complexed with T<sub>3</sub>, Triac, or GC-1 are purified according to the  
17 same procedures described above for the rat TR- $\alpha$  LBD, with the following modifications.

18 The expression of human TR- $\beta$  LBD differs from the rat TR- $\alpha$  LBD in that the  
19 human TR- $\beta$  LBD residues extend from the amino acid at position 716 through the amino  
20 acid at position 1022, according to the amino acid numbering scheme for the various nuclear  
21 receptor LBDs depicted in FIG. 3. FIG. 3 illustrates a numbering scheme applicable to all  
22 of the nuclear receptors listed as well as to any additional homologous nuclear receptors.  
23 The vertical lines on FIG. 3 at position 725 and at position 1025 delineate the preferred  
24 minimum amino acid sequence necessary to obtain adequate binding of ligand. The amino  
25 acid sequence from position 716 to position 1022 according to the numbering scheme of  
26 FIG. 3 corresponds to the amino acid positions 202 to 461 according to the conventional  
27 numbering of the amino acid sequence of human TR- $\beta$  which is publicly available. Also, the  
28 human TR- $\beta$  LBD is expressed with a histidine tag, as described in Crowe *et al.*, *Methods in*  
29 *Molecular Biology* (1994) 31:371-387, incorporated by reference herein.

30 The purification of human TR- $\beta$  LBD is the same as that described above for the rat  
31 TR- $\alpha$  LBD with the following exceptions. First, before the purification step using the

1 hydrophobic interaction column, a step is added in which the expressed human TR- $\beta$  LBD is  
2 purified using a nickel NTA column (commercially available from Qiagen, Chatsworth, CA)  
3 according to manufacturer's instructions, and eluted with 200 mM imidazole. The second  
4 difference is that in the purification of the human TR- $\beta$  LBD, the purification step using a  
5 heparin column is omitted.

6 The crystallization of human TR- $\beta$  LBD bound to T<sub>3</sub>, Triac or GC-1 is as follows.  
7 Crystals are obtained in condition 7 of the factorial screen using hanging drops as before at  
8 ambient temperature (22°C) using the factorial crystallization screening trials of Jancarik &  
9 Kim (1991) and using the commercially available product from Hampton Research,  
10 Riverside). The following are optimum conditions: hexagonal bipyrimidal crystals are  
11 grown at 4°C for 2-3 days from hanging drops containing 1.0-1.2 M sodium acetate (pH  
12 unadjusted) and 0.1 M sodium cacodylate (pH 7.4), 3 mM DTT, with either a 1  $\mu$ l protein  
13 solution, 1  $\mu$ l precipitant solution or 2  $\mu$ l protein solution, 1  $\mu$ l precipitant solution and a 0.6  
14 ml reservoir using silanized coverslip, at a protein concentration of 7-10 mg/ml. The best  
15 crystals have a limiting dimension of 200  $\mu$ m. The following are optimum conditions for  
16 crystallization of the TR- $\beta$  LBD with GC-1: hexagonal bipyrimidal crystals are grown at 4°C  
17 for 2-3 days from hanging drops containing 0.8-1.0M sodium acetate (pH unadjusted), 50-  
18 200nM sodium succinate, and 0.1M sodium cacodylate (pH 7.2), 3mM DTT, 1  $\mu$ l protein  
19 solution, 1  $\mu$ l precipitant solution and a 0.6ml reservoir using silanized coverslip, at a protein  
20 concentration of 7-10 mg/ml. The best crystals have a limiting dimension of 200 $\mu$ M. The  
21 unit cell dimensions are cell length a=b=68.73, cell length c=130.09. The unit cell angles  
22 are  $\alpha=90^\circ$ ,  $\beta=90^\circ$ ,  $\gamma=120^\circ$ .

23 The crystal system for human TR- $\beta$  LBD bound to T<sub>3</sub>, Triac or GC-1 is trigonal with  
24 the space group p3<sub>1</sub>21. The unit cell dimensions are cell length a = cell length b = 68.448  
25 angstroms, cell length c = 130.559 angstroms. The angles are  $\alpha = 90^\circ$ ,  $\beta = 90^\circ$ ,  
26 gamma = 120°.

27

## 28 **EXAMPLE 9 - DETERMINATION OF LIGANDED TR- $\alpha$ LBD AND TR- $\beta$ CRYSTAL** 29 **STRUCTURES**

30 Data from each cocrystal (Rat TR- $\alpha$  LBD with Dimit, T3 and IpBr2; Human TR- $\beta$   
31 LBD with Triac and GC-1) is measured on a Mar area detector at Stanford Synchrotron



1 Radiation Laboratory beamline 7-1 ( $\lambda = 1.08$  angstroms) using  $1.2^\circ$  oscillations. Data from  
2 the cocrystal of the hTR- $\beta$  LBD with Triac is measured on a Mar area detector at Stanford  
3 Synchrotron Radiations Laboratory beamline 7-1 ( $\lambda = 1.08$  angstroms) using  $1.0^\circ$   
4 oscillations. Data from the cocrystal of the hTR- $\beta$  LBD with GC-1 is measured on a R-axis  
5 II area detector on a Rigaku rotating Cu anode (50kV, 300mA). The crystals are transferred  
6 into a cryosolvent containing 1.2M sodium acetate, 0.1M sodium cacodylate, and 15%  
7 glycerol followed by a second transfer into 30% glycerol, then flash frozen in liquid  
8 nitrogen. An orientation matrix for each crystal is obtained using DENZO. The reflections  
9 are integrated with DENZO (commercially available from Molecular Structure Corp., The  
10 Woodlands, Texas) and are scaled with SCALEPACK (as described in Otwinowski, Z,  
11 *Proceedings of the CCP4 Study Weekend: "Data Collection and Processing,"* 56-62 (SERC  
12 Daresbury Laboratory, Warrington, UK 1993) incorporated by reference).

13 For rTR- $\alpha$  cocrystals, data from the  $T_3$  cocrystal is measured with the  $b^*$  axis  
14 approximately parallel with the spindle. The crystals are flash frozen at  $-178^\circ\text{C}$  in a nitrogen  
15 gas stream with the MPD mother liquor serving as the cryosolvent. An orientation matrix  
16 for each crystal is determined using REFIX (Kabsch, W., *J. Appl. Crystallogr.* (1993)  
17 26:795-800 incorporated by reference). Reflections are integrated with DENZO, and are  
18 scaled with SCALEPACK.

19 For the  $T_3$  data set, Bijvoet pairs are kept separate, and are locally scaled using  
20 MADSYS (W. Hendrickson (Columbia University) and W. Weis (Stanford University)).

21 Cocrystals prepared from the three isosteric ligands are isomorphous. MIR analysis is  
22 performed using programs from the CCP4 suite (Collaborative Computational Project, N.R.  
23 *Acta Crystallogr.* (1994) D50:760-763, incorporated by reference herein). Difference  
24 Pattersons is calculated for both  $T_3$  and  $\text{IpBr}_2$ , taking the Dimit cocrystal as the parent. The  
25 positions of the three iodine atoms in the  $T_3$  difference Patterson are unambiguously  
26 determined from the Harker section of the density map as peaks of  $11\sigma$  above background.  
27 The positions for the two bromine atoms in the  $\text{IpBr}_2$  cocrystals, are located independently,  
28 as peaks  $8\sigma$  above the noise level. Phases for the LBD-122/410 are calculated from the  
29 solution to the  $\text{IpBr}_2$  difference Patterson, and are used to confirm the location of the unique  
30 third iodine of the  $T_3$  cocrystal. Halogen positions are refined with MLPHARE, including the  
31 anomalous contributions from the iodine atoms (Otwinowski, Z, *Proceedings of the CCPR*

1 *Study Weekend* 80-86 (SERC Daresbury Laboratory, Warrington, UK 1991)). The MIRAS  
 2 phases are improved through solvent flattening/histogram matching using DM (Cowtan, K.,  
 3 *Joint CCP4 and ESF-EACBM Newsletter on Protein Crystallography* (1994) 31: 34-38,  
 4 incorporated by reference herein).

5 A model of the LBD-122/410 with Dimit bound is built with the program O from the  
 6 solvent flattened MIRAS 2.5 angstrom electron density map (Jones *et al.*, *Acta Crystallogr.*  
 7 (1991) A 47:110-119, incorporated by reference herein). The initial model, without ligand,  
 8 ( $R_{\text{cryst}} = 40.1\%$ ), is refined using least-squares protocols with XPLOR. The Dimit ligand  
 9 is built into unambiguous Fo-Fc difference density during the following round. Subsequent  
 10 refinement employs both least-squares and simulated annealing protocols with XPLOR  
 11 (Brunger *et al.*, *Science* (1987) 235:458-460), incorporated by reference herein). Individual  
 12 atomic B-factors are refined isotropically. As defined in PROCHECK, all residues are in  
 13 allowed main-chain torsion angle regions as described in Laskowski *et al.*, *J. Appl.*  
 14 *Crystallogr.*, (1993) 26:283-291, incorporated by reference herein. The current model is  
 15 missing 34 residues (Met<sub>122</sub>-Gln<sub>156</sub>) at the N-terminus, and 5 residues (Glu<sub>406</sub>-Val<sub>410</sub>) at the C-  
 16 terminus.

17 In addition, the following residues are not modeled beyond C $\beta$  due to poor density:  
 18 184, 186, 190, 198, 206, 209, 240, 301, 330, 337, 340, 343, 359, and 395. The average B-  
 19 value for protein atoms is 34.5 Å<sup>2</sup>. The final model consists of the LBD-122/410, residues  
 20 Arg<sub>157</sub>-Ser<sub>183</sub>, Trp<sub>185</sub>-Gly<sub>197</sub>, Ser<sub>199</sub>-Asp<sub>206</sub> and Asp<sub>208</sub>-Phe<sub>405</sub>; three cacodylate-modified  
 21 cysteines: Cys<sub>334</sub>, Cys<sub>380</sub> and Cys<sub>392</sub>; and 73 solvent molecules modeled as water (2003  
 22 atoms).

$$23 \quad *R_{\text{sym}} = 100 \times \sum_{hkl} \sum_i |I_i - \bar{I}| / \sum_{hkl} \sum_i I_i$$

$$24 \quad \dagger R_{\text{der}} = 100 \times \sum_{hkl} |F_{\text{PH}} - F_{\text{H}}| / \sum_{hkl} |F_{\text{P}}|$$

25 The occupancy for the two bromine sites is set to 35 electrons. The occupancies of the iodine  
 26 sites are relative to this value.

27 §Phasing power =  $\langle FH \rangle / \langle \epsilon \rangle$ , where  $\langle FH \rangle$  is the mean calculated heavy atom structure factor  
 28 amplitude and  $\langle \epsilon \rangle$  is the mean estimated lack of closure.

29 ||R<sub>cullis</sub> =  $\langle \epsilon \rangle / \langle \text{iso} \rangle$ , where  $\langle \epsilon \rangle$  is the mean estimated lack of closure and  $\langle \text{iso} \rangle$  is the  
 30 isomorphous difference.

1  $R_{\text{cryst}} = 100 \times \sum_{hkl} |F_o - F_c| / \sum_{hkl} |F_o|$  where  $F_o$  and  $F_c$  are the observed and calculated  
 2 structure factor amplitudes (for data  $F/\sigma > 2$ ). The  $R_{\text{free}}$  was calculated using 3% of the  
 3 data, chosen randomly, and omitted from the refinement.

4  $\text{Correlation coefficient} = \sum_{hkl} (|F_o| - |F_c|) \times (|F_o| - |F_c|) / \sum_{hkl} (|F_o| - |F_c|)^2 \times \sum_{hkl}$   
 5  $(|F_o| - |F_c|)^2$

6

#### 7 **EXAMPLE 10. PHASING OF THE rTR- $\alpha$ LBD AND hTR- $\beta$ LBD COMPLEX WITH TRIAC**

8 Due to the possible non-isomorphism of the rTR $\alpha$  LBD complex with Triac, a  
 9 molecular replacement solution is determined using AMORE (Navaza, J., *Acta*  
 10 *Crystallographica Section A-Fundamentals of Crystallography* (1994) 50:157-63 from a  
 11 starting model consisting of rTR $\alpha$  LBD complex with T<sub>3</sub>, but with the ligand, all water  
 12 molecules, and the following residues omitted: Asn 179, Arg228, Arg262, Arg266, and Ser  
 13 277. Strong peaks are obtained in both the rotation and translation searches, with no  
 14 significant ( $> 0.5$  times the top peak) false solutions observed (Table 6). Strong positive  
 15 density present in both the anomalous and conventional difference Fourier maps confirm the  
 16 solution. Maps are calculated using sigma-A weighted coefficients output by REFMAC  
 17 (Murshudov, *et al.* "Application of Maximum Likelihood Refinements," in *Refinement of*  
 18 *Protein Structures, Proceedings of Daresbury Study Weekend* (1996)) after 15 cycles of  
 19 maximum likelihood refinement. Triac, the omitted residues, and water molecules 503, 504,  
 20 534 (following the numbering convention for the TR complex with T<sub>3</sub>) are built into the  
 21 resulting difference density using O (Jones *et al.*); the conformations of these residues are  
 22 further confirmed in a simulated-annealing omit map (Brunger *et al.*). The complete model  
 23 is then refined using positional least-squares, simulated annealing, and restrained, grouped B  
 24 factor refinement in XPLOR to an  $R_{\text{cryst}}$  of 23.6% and an  $R_{\text{free}}$  of 24.1%

25 Phasing of a related LBD using the structure of the rTR- $\alpha$  LBD is conducted as  
 26 follows. A molecular replacement solution for the hTR- $\beta$  LBD complex with Triac is  
 27 determined using AMORE from a starting model consisting of the rTR- $\alpha$  LBD complexed  
 28 with T<sub>3</sub>, but with the ligand and all water molecules omitted. Strong peaks are obtained in  
 29 both the rotation and translation searches, with no significant ( $> 0.5$  times the top peak) false  
 30 solutions (Table 7). Strong positive density present in both the anomalous and conventional  
 31 difference Fourier maps confirm the solution. Initial maps are calculated using sigma-A

1 weighted coefficients output by REFMAC after 9 cycles of maximum likelihood refinement.  
 2 The real-space fit for each residues was calculated using OOPS (Kleywegt, GJ and Jones.  
 3 TA, OOPS-a-daisy, ESF/CCP4 Newsletter 30, June 1994, pp. 20-24) and the residues with a  
 4 real-space fit less than 2 standard deviations below the mean removed: Ala253-Lys263;  
 5 Glu245-Leu250. To reduce bias, the following residues were modeled as alanine: Arg282,  
 6 Arg316, Arg 320, Asn 331. Cycles of rebuilding and positional least-squares, simulated  
 7 annealing, and restrained, grouped B factor refinement with XPLOR produce a model with  
 8 an  $R_{\text{cryst}}$  of 25.3 and an  $R_{\text{free}}$  of 28.9%. The final model consists of hTR- $\beta$  LBD residues  
 9 Glu202-Gln252, Val264-Glu460; three cacodylate-modified cysteines with the cacodylate  
 10 moiety modeled as free arsenic: Cys294, Cys298, Cys388, and Cys434; and 35 solvent  
 11 molecules modeled as water.

### 13 **EXAMPLE 11. CONNECTING QSAR WITH STRUCTURE IN THE THYROID HORMONE** 14 **RECEPTOR**

15 The conclusions of classic thyroid hormone receptor quantitative structure-activity  
 16 relationships may be summarized as follows:

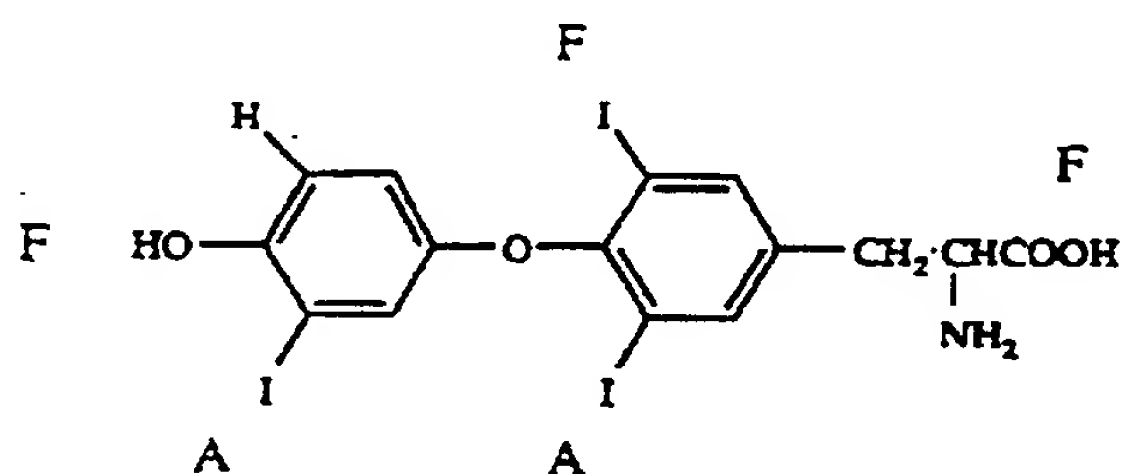
- 17 1) the  $R_4$ '-hydroxyl group functions as a hydrogen bond donor;
- 18 2) the amino-propionic acid interacts electrostatically through the carboxylate  
 19 anion with a positively charged residue from the receptor;
- 20 3) the preferences of  $R_3/R_5$  substituent are  $I > Br > Me > > H$ ;
- 21 4) the preferences of the  $R_3$ '-substituent are  $Ipr > I > Br > Me > > H$ .

22 The structure of the thyroid hormone receptor ligand binding domain complexed with the  
 23 agonists T3, IpBr<sub>2</sub>, Dimit, Triac, and GC1 as provided herein, permits:

- 24 1) the identification of receptor determinants of binding at the level of the  
 25 hydrogen bond;
- 26 2) the association of these determinants with the predictions of classic thyroid  
 27 hormone receptor QSAR; and
- 28 3) prediction as to which determinants of binding are rigid, and which are  
 29 flexible, for both the ligand and the receptor.

30 This classification for the agonists of the type ( $R_1$ =amino-propionic, acetic acid;  
 31  $R_3, R_5=I, Br, Me$ ;  $R_3'=Ipr, I$ ) is given below (for the representative ligand T<sub>3</sub>);

1 F = Fiducial (always satisfied)  
 2 A = Adjustable



Based upon the methods and data described herein, the following is an embodiment of the computational methods of the invention, which permit design of nuclear receptor ligands based upon interactions between the structure of the amino acid residues of the receptor LBD and the four different ligands described herein. The small molecule structures for the ligands can be obtained from Cambridge Structural Database (CSD), and three dimensional models can be constructed using the methods described throughout the specification. The following are factors to consider in designing synthetic ligands:

1) Histidine 381 acts as a hydrogen bond acceptor for the  $R_4'$  hydroxyl, with the optimal tautomer maintained by water molecules. See FIG. 23 and FIG 24. Histidine is the only hydrophilic residue in this hydrophobic pocket that surrounds the  $R_4'$  substituent. Histidine can be either a hydrogen bond acceptor or donor, depending on its tautomeric state. It is preferably a hydrogen bond donor, but can tolerate being a hydrogen bond acceptor, as for example, when there is a methoxy at the  $R_4'$  position of the ligand;

2) Arginines 228, 262, and 266 interact directly and through water-mediated hydrogen bonds with the  $R_1$ -substituent, with the electrostatic interaction provided by Arginine 266 (as in the Triac complex). This polar pocket is illustrated by FIG. 23 - FIG. 25. FIG. 23 depicts  $T_3$  in the  $TR\alpha$  ligand binding cavity, where  $T_3$ 's amino-propionic  $R_1$ -substituent interacts with Arg 228, HOH5O2, H9H5O3 and HOH5O4 via hydrogen bonds. FIG. 24 depicts Triac in the ligand binding cavity, with its -COOH  $R_1$  substituent in the polar pocket. In FIG. 24, Arg 228 no longer shares a hydrogen bond with the ligand, but the -COOH  $R_1$  substituent forms hydrogen bonds with Arg 266. FIG. 25 superimposes  $T_3$



1 and Triac in the ligand binding cavity and shows several positionally unchanged amino acids  
2 and water molecules, and selected changed interacting amino acids and water molecules.  
3 The three figures illustrate parts of the polar pocket that can change and those parts that do  
4 not move upon binding of different ligands. For example, the Arg 262 at the top of the  
5 polar pocket does not move, even when the  $R_1$  substituent has changed from a -COOH to an  
6 aminopropionic acid group. However, the other two Arginines, Arg 228 and Arg 266,  
7 demonstrate flexibility in the polar pocket to respond to the change in the size or chemical  
8 nature of the  $R_1$  substituent.

9       3) Inner and outer pockets for the  $R_3/R_5$  substituents are formed by Ser260,  
10 Ala263, Ile299; and Phe 218, Ile221, Ile222, respectively. See FIGS. 21 and 22. The  
11 inner pocket is filled by either the  $R_3$  or the  $R_5$  substituent, regardless of the size of the  
12 substituent, and may act as a binding determinant by positioning the ligand in the receptor.  
13 Optimally, the inner pocket amino acids interact with an  $R_3$  or  $R_5$  substituent that is no  
14 larger than an iodo group. If the inner pocket is filled by the  $R_3$  substituent, then the outer  
15 pocket interacts with the  $R_5$  substituent and vice versa. The outer pocket can adjust to the  
16 size of its substituent through main chain motion centered at the break in helix 3 (Lys220-  
17 Ile221), suggesting that the bending of H3, and motion of the N-terminal portion of H3, may  
18 represent a conformational change induced on ligand binding. The outer pocket has greater  
19 flexibility than does the inner pocket in terms of accommodating a larger substituent group.

20       4) A pocket for the  $R_3'$ -substituent is formed by Phe 215, Gly290, Met388. The  
21 pocket is incompletely filled by the  $R_3'$ -iodo substituent, and accommodates the slightly  
22 larger 3'-isopropyl substituent by movement of the flexible Met388 side chain and the H7/H8  
23 loop. This pocket can accommodate  $R_3'$  substituents that are even larger than isopropyl, for  
24 example, a phenyl group.

25       The above information will facilitate the design of high affinity agonists and  
26 antagonists by improving automated QSAR methodologies and informing manual modeling of  
27 pharmaceutical lead compounds. For example, the inclusion of discrete water molecules  
28 provides a complete description of hydrogen bonding in the polar pocket for use with  
29 pharmacophore development; also, the identification of mobile and immobile residues within  
30 the receptor suggests physically reasonable constraints for use in molecular  
31 mechanics/dynamics calculations.

## 1 EXAMPLE 12. DESIGN OF AN INCREASED AFFINITY LIGAND

2 Direct interaction between the receptor and the ligand is limited in the polar pocket,  
3 which interacts with the  $R_1$  substituent. While the lack of complementarity may contain  
4 implications for biological regulation, it also provides an opportunity for increasing affinity  
5 by optimizing the interaction between the amino acids of the polar pocket and the  $R_1$   
6 substituent of a synthetic ligand. The structure of the receptor-ligand interactions described  
7 herein enables design of an increased affinity synthetic ligand having two complementary  
8 modifications:

9 1) Remove the positively charged amine. The strongly positive electrostatic  
10 potential predicted for the polar pocket suggests that the positively charged amine of the  
11 aminopropionic acid  $R_1$  substituent may be detrimental to binding. Suitable groups for  
12 substitution are suggested by the nature of nearby hydrogen bond partners: for example, Thr  
13 275 O or Ser 277 N. See e.g. Tables in Appendix 2. For example, any negatively  
14 charged substituent would be compatible for interacting with the amino acids of the polar  
15 pocket, including carboxylates, carbonyl, phosphonates, and sulfates, comprising 0 to 4  
16 carbons. Another example of an  $R_1$  substitution is an oxamic acid that replaces the amine of  
17 the naturally occurring ligand with one or more carbonyl groups.

18 2) Incorporate hydrogen bond acceptor and donor groups into the  $R_1$ -substituent  
19 to provide broader interactions with the polar pocket scaffold. Such hydrogen bond acceptor  
20 and donor groups incorporated into the  $R_1$ -substituent will allow interactions that would  
21 otherwise occur with water molecules in the polar pocket. Specific waters include HOH 504  
22 (hydrogen bonds with Ala 225 O and Arg 262 NH); and HOH 503 hydrogen bonds with Asn  
23 179 OD1, Ala 180 N), both of which are present in all four complexes (TR LBD complexed  
24 with T3, TR LBD complexed with IpBr<sub>2</sub>, TR LBD complexed with Dimit and TR LBD  
25 complexed with Triac). Analysis of the hydrogen bonding network in the polar pocket  
26 suggests replacement of HOH 504 with a hydrogen bond acceptor, and HOH 503 with an  
27 hydrogen bond donor (although the chemical nature of asparagine probably permits flexibility  
28 at this site). Thus, incorporating a hydrogen bond acceptor in an  $R_1$  substituent that could  
29 take the place of the HOH504 or incorporating a hydrogen bond acceptor in an  $R_1$   
30 substituent that could positionally replace the HOH503, or a combination thereof, are  
31 methods of designing novel synthetic TR ligands.

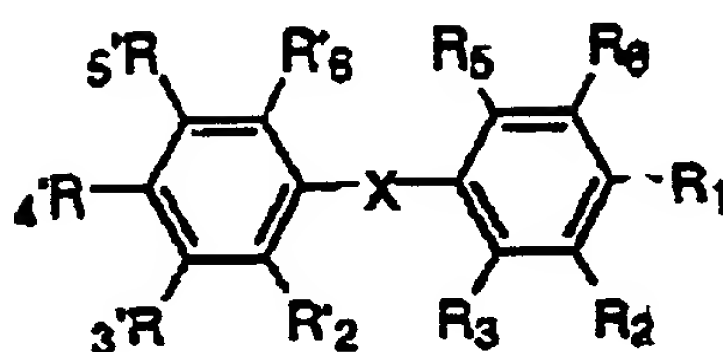
1        These two design approaches can be used separately or in combination to design  
2 synthetic ligands, including those in Table 5 (below).

3        A corollary to this approach is to design specific interactions to the residues Arg262  
4 and Asn 179. The goal is to build in interactions to these residues by designing ligands that  
5 have R<sub>1</sub> substituents that form hydrogen bonds with water molecules or charged residues in  
6 the polar pocket.

7        High-affinity ligands also may be designed and selected using small molecules that  
8 bind to proximal subsites of the target nuclear hormone receptor that are identified in a  
9 structure-based screen and then linked together in their experimentally determined bound  
10 orientations. Such a method has been described in design of high-affinity ligands for the  
11 FK506 binding protein (FKBP), stromelysin, gelatinase A, and human papillomavirus E2  
12 (Hajduk *et al.*, *Science* 278:497-499 (1997)), which reference and its references are  
13 incorporated herein by reference. The preferred small molecules for screening are  
14 compounds of Formula I or derivatives thereof. For example, a compound of Formula I ( $\phi$ -  
15 X- $\phi$ ) or a derivative thereof ( $\phi$ -X or X- $\phi$ ) is screened for binding a target nuclear hormone  
16 receptor LBD. Proximal subsites of the nuclear hormone receptor include the hydrophobic  
17 and polar pockets of the LBD, and substites extended therefrom. As an example, Fourier  
18 transformation or nuclear magnetic resonance (NMR) -based structure screens can be used.  
19 When a NMR-based screen is used, binding can be detected from the amide chemical shift  
20 changes observed in two-dimensional heteronuclear single quantum correlation (HSQC)  
21 spectra aquired in the presence and absence of added compound. Once two ligands are  
22 identified that bind to the receptor, the crystal or solution structure of the ternary complex is  
23 determined. From the structural information, a compound is synthesized which links the two  
24 ligands, where the linker is selected based on structural information. The new compound is  
25 then screened for binding affinity, for example, using a binding assay as described herein.  
26 Only a few linked ligands need to synthesized and screened when using this approach.

27        Compounds of the invention also may be iteratively designed from structural  
28 information of the compounds described above using other structure-based design/modeling  
29 techniques (Jackson, R.C., *Contributions of protein structure-based drug design to cancer*  
30 *chemotherapy. Seminars in Oncology*, 1997, 24(2)L164-172; and Jones, T.R., *et al.*, *J.*  
31 *Med. Chem.*, 1996 39(4):904-917).

Table 5: Synthetic TR Ligands



R1	R2	R3	R5	R6	X	R'2	R'3	R'4	R'5	R'6
CO2H	H	Me	Me	H	O	H	Me	OH	Me	H
CH2CO2H		I	I		S		Et	SH	Et	
CH2CH2CO2H		Br	Br				nPr	NH2	nPr	
CH2CH(NH2)CO2H		Cl	Cl				iPr		iPr	
OCH2CO2H		Et	Et				Ph		nBu	
OCH2CH2CO2H		OH	OH				I		nPen	
NHCH2CO2H		NH2	NH2				Br		nHex	
NHCH2CH2CO2H		SH	SH				Cl		Ph	
CH2COCOCO2H									hetero	
									cycle	
NHCOCOCO2H									aryl	
COCO2H										
CF2CO2H										
COCH2CO2H										

Any combination of the above substituents in the biphenyl ether scaffold structure shown above may result in a potentially pharmacologically useful ligand for the thyroid hormone receptor. These novel ligands may be antagonists of the thyroid receptor.

TABLE 6: TR- $\alpha$  LBD-122/410

	Dimit	T3	IpBr <sub>2</sub>	Triac
1				
2				
3	<b>Data collection</b>			
4	<b>Cell dimensions</b>			
5	a (Å)	117.16	117.19	117.18
6	b (Å)	80.52	80.20	80.12
7	c (Å)	63.21	63.23	63.13
8	$\beta$ (°)	120.58	120.60	120.69
9	Resolution (Å)	2.2	2.0	2.1
10	Obs. Reflections, (no.)	57031	64424	66877
11	Unique Reflections,	22327	21023	23966
12	(no.)			
13	Completeness, (%)	87.0	82.4	93.7
14	*R <sub>sym</sub> (%)	3.9	3.5	4.5
15	<b>Phasing (15.0 - 2.5Å)</b>			
16	†R <sub>der</sub> (%)	-	19.6	11.6
17	No. of sites	-	3	2
18	‡Occupancy	-	44.6 (19.8)	35.0
19	(Anomalous)	-	50.2 (23.7)	35.0
20			39.2 (22.3)	
21	§F <sub>H</sub> /E			
22	centric (acentric)			
23	15.0-5.0 Å	-	3.67 (4.61)	2.25 (3.09)
24	5.0-3.0 Å	-	2.23 (2.75)	1.25 (1.85)
25	3.0-2.5 Å	-	1.64 (1.99)	1.15 (1.57)
26	IR <sub>Cullis</sub> (%)			
27	15.0-5.0 Å	-	33	44
28	5.0-3.0 Å	-	45	63
29	3.0-2.5 Å	-	60	65
30	Mean figure of merit	0.62	-	-
31	MR Phasing			
32	(10-3.5Å)			
33	Rotation Search:			$\Theta_1 = 309.37$
34	Euler Angles (°)			$\Theta_2 = 48.96$
35				$\Theta_3 = 127.28$
36	§ correlation coefficient			34.3
37	Translation Search:			x = 0.1571
38	Fractional coordinates			
39				y = 0.000



$z = 0.3421$

65.8

31.2

25-2.5

23.6

24.1

**TABLE 7: TR- $\beta$  LBD-202/461**

	Triac	T3	GC1
13 Data collection			
14 Space Group		P3121	
15 Cell dimensions			
16 a (Å)	68.9	68.45	68.73
17 c (Å)	131.5	130.56	130.09
18 Resolution (Å)	2.4	3.1	2.8
19 Obs. Reflections, (no.)	80196	55103	54104
20 Unique Reflections, (no.)	14277	6847	8987
21 Coverage (%)	97.0	95.7	97.1
22 *R <sub>sym</sub> (%)	5.1	4.6	5.5
23 MR Phasing (15.0 - 3.5 Å)			
24 Rotation Search	$\Theta_1=39.13$		
25 Euler Angles (°)	$\Theta_2=68.00$		
26	$\Theta_3=323.6$		
27 § correlation coefficient	21.6		
28 (Highest false peak)	(10.8)		
29 Translation Search	x=0.748		
30 Fractional Coordinates	y=0.158		
31	z=0.167		
32 § correlation coefficient	57.5		
33 (Highest false peak)	(38.7)		
34	0.612		
35 *R factor	40.7	40.8	
36 Refinement			
37 Resolution (Å)	30-2.4		30-2.9
38 $R_{cryst}$ (%)	25.3		27.3
39 $R_{free}$ (%)	28.9		33.4

1  
2 All publications and patent applications mentioned in this specification are herein  
3 incorporated by reference to the same extent as if each individual publication or patent  
4 application was specifically and individually indicated to be incorporated by reference. The  
5 nuclear receptor ligands, particularly the TR ligands, of these references are herein  
6 incorporated by reference and can be optionally excluded from the claimed compounds with a  
7 proviso.

8 Headings and subheadings are presented only for the convenience of the reader and  
9 should not be used to construe the meaning of terms used within such headings and  
10 subheadings.

11 The invention now being fully described, it will be apparent to one of ordinary skill -  
12 in the art that many changes and modifications can be made thereto without departing from  
13 the spirit or scope of the appended claims.

1 WHAT IS CLAIMED IS:

2

3 1. A method of modulating the activity of a thyroid hormone receptor (TR) which  
4 comprises administering to a mammal in need thereof a compound of the formula:

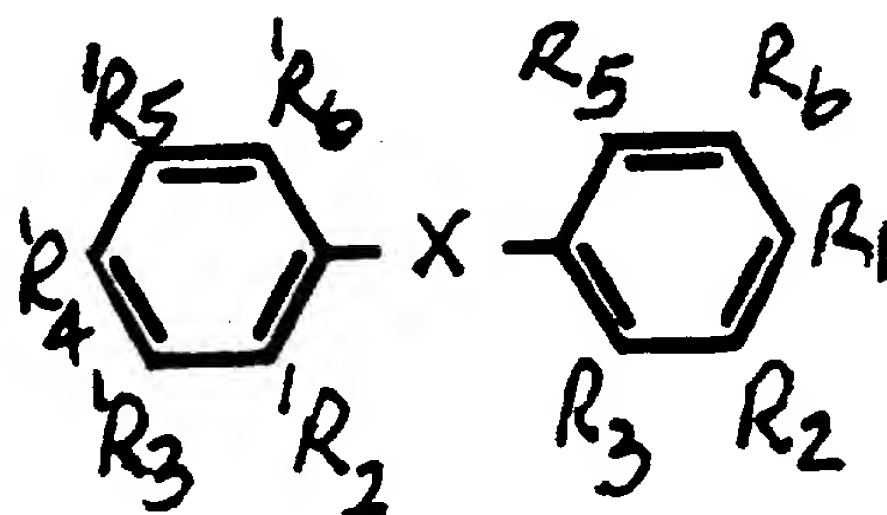
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wherein said compound fits spatially and preferentially into a TR ligand binding domain (TR LBD) and comprises the following substituents:

(i) an R1-substituent comprising an anionic group that interacts with a side chain nitrogen atom of an arginine corresponding to a residue selected from the group consisting of Arg228, Arg262, and Arg266 of human TR- $\alpha$ , and Arg282, Arg316 and Arg320 of human TR- $\beta$ , and wherein the anionic group is 1.7-4.0Å from the nitrogen atom;

(ii) an R2-substituent comprising a hydrophobic or hydrophilic group that fits spatially into the TR LBD;

(iii) an R3-substituent comprising a hydrophobic or hydrophilic group that interacts with a side chain atom of a serine, alanine or isoleucine corresponding to a residue selected from the group consisting of Ser260, Ala263 and Ile299 of human TR- $\alpha$ , and Ser314, Ala317 and Ile352 of human TR- $\beta$ , and wherein the hydrophobic or hydrophilic group is 1.7-4.0Å from the side chain atom;

1 (iv) an R5-substituent comprising a hydrophobic or hydrophilic group that interacts  
2 with a side chain atom of a phenylalanine or isoleucine corresponding to a residue selected  
3 from the group consisting of Phe218, Ile221 and Ile222 of human TR- $\alpha$ , and Phe272, Ile275  
4 and Ile276 of human TR- $\beta$ , and wherein the hydrophobic or hydrophilic group is 1.7-4.0Å  
5 from the side chain atom;

6 (v) an R6-substituent comprising a hydrophobic or hydrophilic group that fits  
7 spacially into the TR LBD;

8 (vi) an X-substituent comprising a hydrophobic or hydrophilic group that interacts  
9 with a side chain atom of a leucine corresponding to a residue selected from the group  
10 consisting of Leu276 and Leu292 of human TR- $\alpha$ , and Leu 330 and Leu346 of human TR- $\beta$ ,  
11 and wherein the hydrophobic or hydrophilic group is 1.7-4.0Å from the side chain atom;

12 (vii) an R2'-substituent comprising a hydrophobic or hydrophilic group that fits  
13 spacially into the TR LBD;

14 (viii) an R3'-substituent comprising a hydrophobic group that interacts with a side  
15 chain atom of a phenylalanine, glycine or methionine corresponding to a residue selected  
16 from the group consisting of Phe215, Gly290, and Met388 of human TR- $\alpha$ , and Phe269,  
17 Gly344, Met442 of human TR- $\beta$ , and wherein the hydrophobic group is 1.7-4.0Å from the  
18 side chain atom;

19 (ix) an R4'-substituent comprising an hydrogen bond donor or acceptor group that  
20 interacts with a side chain carbon or nitrogen atom of a histidine corresponding to residue  
21 His381 of human TR- $\alpha$ , and His435 of human TR- $\beta$ , and wherein the hydrogen bond donor  
22 or acceptor group is 1.7-4.0Å from the side chain atom;

(x) an R5'-substituent comprising a hydrophobic or hydrophilic group that fits  
spacially into the TR LBD;

(xi) and R6'-substituent comprising a hydrophobic or hydrophilic group that fits  
spacially into the TR LBD;

wherein said compound is other than a thyronine or thyronine-like compound  
disclosed in a reference cited in Appendix I, and wherein the activity of said TR is  
modulated.

2. The method according to claim 1,

wherein R<sub>1</sub> is

-O-CH<sub>2</sub>CO<sub>2</sub>H, -NHCH<sub>2</sub>CO<sub>2</sub>H,

-CO<sub>2</sub>H, -CH<sub>2</sub>CO<sub>2</sub>H, -CH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H, -CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H,

-CH<sub>2</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H, -CH<sub>2</sub>CH[NHCOCH<sub>2</sub>]<sub>2</sub>CO<sub>2</sub>H, -CH<sub>2</sub>CH[NHCO(CH<sub>2</sub>)<sub>15</sub>CH<sub>3</sub>

]CO<sub>2</sub>H, -CH<sub>2</sub>CH[NH-FMOC]CO<sub>2</sub>H, -CH<sub>2</sub>CH[NH-tBOC]CO<sub>2</sub>H, or a carboxylate

connected to the ring with a 0 to 3 carbon linker,

-PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>CH<sub>2</sub>PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>CHNH<sub>2</sub>PO<sub>3</sub>H<sub>2</sub>,

-CH<sub>2</sub>CH[NHCOCH<sub>2</sub>]<sub>2</sub>PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>CH[NHCO(CH<sub>2</sub>)<sub>15</sub>CH<sub>3</sub>]PO<sub>3</sub>H<sub>2</sub>,

-CH<sub>2</sub>CH[NH-FMOC]PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>CH[NH-tBOC]PO<sub>3</sub>H<sub>2</sub>, or a phosphate or

phosphonate connected to the ring with a 0 to 3 carbon linker,

-SO<sub>3</sub>H, -CH<sub>2</sub>SO<sub>3</sub>H, -CH<sub>2</sub>CH<sub>2</sub>SO<sub>3</sub>H, -CH<sub>2</sub>CHNH<sub>2</sub>SO<sub>3</sub>H, -CH<sub>2</sub>CH[NHCOCH<sub>2</sub>]<sub>2</sub>SO<sub>3</sub>H,

-CH<sub>2</sub>CH[NHCO(CH<sub>2</sub>)<sub>15</sub>CH<sub>3</sub>]SO<sub>3</sub>H, -CH<sub>2</sub>CH[NH-FMOC]SO<sub>3</sub>H, -CH<sub>2</sub>



1 CH[NH-tBOC]SO<sub>3</sub>H, or a sulfate or sulfite connected to the ring with a 0 to 3 carbon  
2 linker,

3  
4 or acts as the functional equivalent of CH<sub>2</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H of T3 in the molecular  
5 recognition domain when bound to a TR, wherein said R<sub>1</sub> can be optionally  
6 substituted with an amine,

7  
8 wherein R<sub>2</sub> is

9 H, halogen, CF<sub>3</sub>, OH, NH<sub>2</sub>, SH, CH<sub>3</sub>, -Et,

10 or acts as the functional equivalent of H in the molecular recognition domain when  
11 bound to a TR,

12  
13 wherein R<sub>3</sub> is

14 -H, halogen, -CF<sub>3</sub>, -OH, -NH<sub>2</sub>, -N<sub>3</sub>, -SH, -CH<sub>3</sub>, -Et,

15 or acts as the functional equivalent of I in the molecular recognition domain when  
16 bound to a TR,

17  
18 wherein R<sub>5</sub> is

19 -H, halogen, -CF<sub>3</sub>, -OH, -NH<sub>2</sub>, -N<sub>3</sub>, -SH, -CH<sub>3</sub>, -Et, or acts as the functional  
20 equivalent of I in the molecular recognition domain when bound to a TR, and R<sub>3</sub> can  
21 be identical to R<sub>5</sub>,

22  
23 wherein R<sub>6</sub> is

1 -H, halogen, -CF<sub>3</sub>, -OH, -NH<sub>2</sub>, -SH, -CH<sub>3</sub>, or acts as the functional equivalent of H  
2 in the molecular recognition domain when bound to a TR, and R<sub>2</sub> can be identical to  
3 R<sub>6</sub>,

4  
5 wherein R<sub>2</sub>' is

6 -H, halogen, -CF<sub>3</sub>, -OH, -NH<sub>2</sub>, -N<sub>3</sub>, -SH, -CH<sub>3</sub>, -Et, or acts as the functional  
7 equivalent of H in the molecular recognition domain when bound to a TR,

8  
9 wherein R<sub>3</sub>' is any hydrophobic group, including

10 halogen, -CF<sub>3</sub>, -SH, alkyl, aryl, 5- or 6-membered heterocyclie, cyano, or acts as the  
11 functional equivalent of I in the molecular recognition domain when bound to a TR,

12  
13 wherein R<sub>4</sub>' is

14 -H, halogen, -CF<sub>3</sub>, -OH, -NH<sub>2</sub>, NH<sub>3</sub>, -N(CH<sub>3</sub>)<sub>3</sub>, carboxylate, phosphonate, phosphate  
15 or sulfate, -SH, -CH<sub>3</sub>, -Et, or akyl, aryl or 5- or 6-membered heterocyclic aromatic  
16 attached through urea or carbamate linkages to O or N or S at the R<sub>4</sub>' position, or  
17 acts as the functional equivalent of OH in the molecular recognition domain when  
18 bound to a TR,

19  
20 wherein R<sub>5</sub>' is

21 -H, -OH, -NH<sub>2</sub>, -N(CH<sub>3</sub>)<sub>2</sub> -SH -NH<sub>3</sub>, -N(CH<sub>3</sub>)<sub>3</sub>, carboxylate, phosphonate, phosphate,  
22 sulfate, branched or straight chain alkyl having 1 to 9 carbons, substituted or  
23 unsubstituted aryl, wherein said substituted aryl is substituted with halogen or 1 to 5

1 carbon alkyl and wherein said aryl is optionally connected to the ring by a -CH<sub>2</sub>-,  
2 aromatic heterocycle having 5 to 6 atoms, wherein said heterocycle may be substituted  
3 with one or more groups selected from -OH, -NH<sub>2</sub>, -SH, -NH<sub>3</sub>, -N(CH<sub>3</sub>)<sub>3</sub>,  
4 carboxylate, phosphonate, phosphate or sulfate, heteroalkyl, arylalkyl, heteroaryl  
5 alkyl, polyaromatic, or polyheteroaromatic, wherein said R<sub>5</sub>' may be substituted with  
6 polar or charged groups,

7  
8 wherein R<sub>6</sub>' is

9 -H, halogen, -CF<sub>3</sub>, -OH, -NH<sub>2</sub>, -SH, -CH<sub>3</sub>, -Et, or acts as the functional equivalent of  
10 H in the molecular recognition domain when bound to a TR,

11  
12 wherein X is

13 O, S, SO<sub>2</sub>, NH, NR<sub>7</sub>, CH<sub>2</sub>, CHR<sub>7</sub>, CR<sub>7</sub>R<sub>7</sub>, wherein R<sub>7</sub> is alkyl, aryl or 5- or  
14 6-membered heterocyclic aromatic,

15  
16 and wherein said TR LBD ligand has an apparent K<sub>d</sub> for binding TR LBD of 1 μM or less.

17  
18 3. The method of claim 2, wherein

19 R<sub>1</sub> is carboxylate, phosphonate, phosphate or sulfite and is connected to the  
20 ring with a 0 to 3 carbon linker,

21 R<sub>2</sub> is H,

22 R<sub>3</sub> is -I, -Br, or -CH<sub>3</sub>,

23 R<sub>5</sub> is -I, -Br, or -CH<sub>3</sub>,

1  $R_6$  is H,

2  $R_2'$  is H,

3  $R_3'$  is -I, -Br, -CH<sub>3</sub>, -iPr, -phenyl, benzyl, or 5- or 6-membered ring

4 heterocycles,

5  $R_4'$  is -OH, -NH<sub>2</sub>, and -SH,

6  $R_5'$  is -H, -OH, -NH<sub>2</sub>, -N(CH<sub>3</sub>)<sub>2</sub> -SH -NH<sub>3</sub>, -N(CH<sub>3</sub>)<sub>3</sub>, carboxylate,

7 phosphonate, phosphate, sulfate, branched or straight chain alkyl having 1 to 9

8 carbons, substituted or unsubstituted aryl, wherein said substituted aryl is substituted

9 with halogen or 1 to 5 carbon alkyl and wherein said aryl is optionally connected to

10 the ring by a -CH<sub>2</sub>-, aromatic heterocycle having 5 to 6 atoms, wherein said

11 heterocycle may be substituted with one or more groups selected from -OH, -NH<sub>2</sub>, -

12 SH, -NH<sub>3</sub>, -N(CH<sub>3</sub>)<sub>3</sub>, carboxylate, phosphonate, phosphate or sulfate, heteroalkyl,

13 arylalkyl, heteroaryl alkyl, polyaromatic, or polyheteroaromatic, wherein said  $R_5'$

14 may be substituted with polar or charged groups, and

15  $R_6'$  is H.

16  
17 4. The method of claim 1, wherein said compound fits spatially and preferentially  
18 into TR LBD isoform  $\alpha$  (TR- $\alpha$ ).  
19

20 5. The method of claim 4, wherein said compound comprises an anionic group  
21 that interacts with the side chain oxygen or carbon of a serine residue corresponding to  
22 Ser277 of human TR- $\alpha$ , and wherein the anionic group is 1.7-4.0Å from the side chain atom.  
23

1           6.     The method of claim 1, wherein said compound fits spatially and preferentially  
2 into TR LBD isoform  $\beta$  (TR- $\beta$ ).

3  
4           7.     The method of claim 6, wherein said compound comprises an anionic group  
5 that interacts with the side chain nitrogen of an arginine corresponding to Asn331 of human  
6 TR- $\beta$ , and the anionic group is 1.7-4.0Å from the side chain atom.

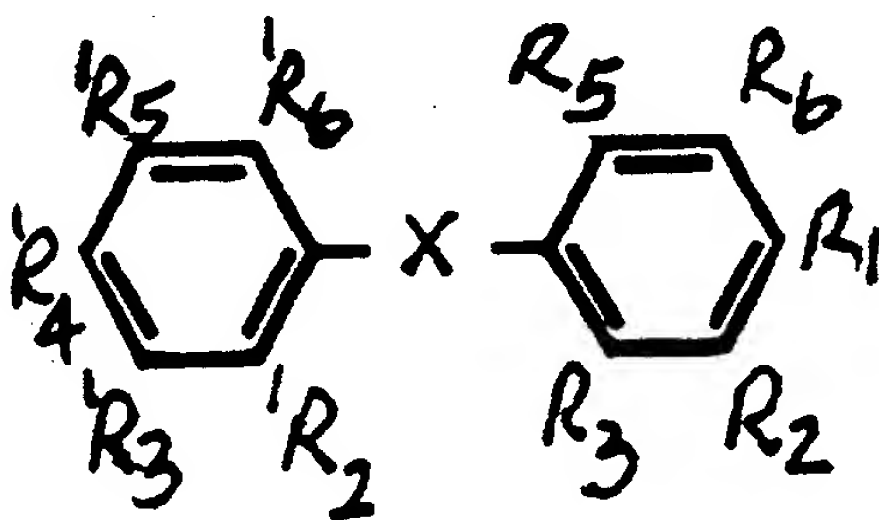
7  
8           8.     A method for identifying a compound capable of selectively modulating the  
9 activity of a thyroid hormone receptor (TR) isoform, said method comprising:

10           modeling test compounds that fit spacially and preferentially into a TR ligand  
11 binding domain (TR LBD) isoform of interest using an atomic structural model of a TR LBD  
12 isoform bound to a test compound,

13           screening said test compounds in a biological assay for TR isoform activity  
14 characterized by binding of a test compound to a TR LBD isoform, and

15           identifying a test compound that selectively modulates the activity of a TR  
16 isoform.

17  
18           9.     The method of claim 8, wherein said compound is of the formula:





1 which comprises the following substituents:

2 (i) an R1-substituent comprising an anionic group that interacts with a side chain  
3 nitrogen atom of an arginine corresponding to a residue selected from the group consisting of  
4 Arg228, Arg262, and Arg266 of human TR- $\alpha$ , and Arg282, Arg316 and Arg320 of human  
5 TR- $\beta$ , and wherein the anionic group is 1.7-4.0Å from the nitrogen atom;

6 (ii) an R2-substituent comprising a hydrophobic or hydrophilic group that fits  
7 spacially into the TR LBD;

8 (iii) an R3-substituent comprising a hydrophobic or hydrophilic group that  
9 interacts with a side chain atom of a serine, alanine or isoleucine corresponding to a residue  
10 selected from the group consisting of Ser260, Ala263 and Ile299 of human TR- $\alpha$ , and  
11 Ser314, Ala317 and Ile352 of human TR- $\beta$ , and wherein the hydrophobic or hydrophilic  
12 group is 1.7-4.0Å from the side chain atom;

13 (iv) an R5-substituent comprising a hydrophobic or hydrophilic group that interacts  
14 with a side chain atom of a phenylalanine or isoleucine corresponding to a residue selected  
15 from the group consisting of Phe218, Ile221 and Ile222 of human TR- $\alpha$ , and Phe272, Ile275  
16 and Ile276 of human TR- $\beta$ , and wherein the hydrophobic or hydrophilic group is 1.7-4.0Å  
17 from the side chain atom;

18 (v) an R6-substituent comprising a hydrophobic or hydrophilic group that fits  
19 spacially into the TR LBD;

20 (vi) an X-substituent comprising a hydrophobic or hydrophilic group that interacts  
21 with a side chain atom of a leucine corresponding to a residue selected from the group  
22 consisting of Leu276 and Leu292 of human TR- $\alpha$ , and Leu 330 and Leu346 of human TR- $\beta$ ,  
23 and wherein the hydrophobic or hydrophilic group is 1.7-4.0Å from the side chain atom;

(vii) an R2'-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD;

(viii) an R3'-substituent comprising a hydrophobic group that interacts with a side chain atom of a phenylalanine, glycine or methionine corresponding to a residue selected from the group consisting of Phe215, Gly290, and Met388 of human TR- $\alpha$ , and Phe269, Gly344, Met442 of human TR- $\beta$ , and wherein the hydrophobic group is 1.7-4.0Å from the side chain atom;

(ix) an R4'-substituent comprising an hydrogen bond donor or acceptor group that interacts with a side chain carbon or nitrogen atom of a histadine corresponding to residue His381 of human TR- $\alpha$ , and His435 of human TR- $\beta$ , and wherein the hydrogen bond donor or acceptor group is 1.7-4.0Å from the side chain atom;

(x) an R5'-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD; and

(xi) and R6'-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD.

10. The method according to claim 9,

wherein R<sub>1</sub> is

-O-CH<sub>2</sub>CO<sub>2</sub>H, -NHCH<sub>2</sub>CO<sub>2</sub>H,

-CO<sub>2</sub>H, -CH<sub>2</sub>CO<sub>2</sub>H, -CH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H, -CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H,

-CH<sub>2</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H, -CH<sub>2</sub>CH[NHCOCH $\phi$ <sub>2</sub>]CO<sub>2</sub>H, -CH<sub>2</sub>CH[NHCO(CH<sub>2</sub>)<sub>15</sub>CH<sub>3</sub>

]CO<sub>2</sub>H, -CH<sub>2</sub>CH[NH-FMOC]CO<sub>2</sub>H, -CH<sub>2</sub>CH[NH-tBOC]CO<sub>2</sub>H, or a carboxylate

connected to the ring with a 0 to 3 carbon linker,

1 -PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>CH<sub>2</sub>PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>CHNH<sub>2</sub>PO<sub>3</sub>H<sub>2</sub>,  
2 -CH<sub>2</sub>CH[NHCOCH<sub>2</sub>]<sub>2</sub>PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>CH[NHCO(CH<sub>2</sub>)<sub>15</sub>CH<sub>3</sub>]PO<sub>3</sub>H<sub>2</sub>,  
3 -CH<sub>2</sub>CH[NH-FMOC]PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>CH[NH-tBOC]PO<sub>3</sub>H<sub>2</sub>, or a phosphate or  
4 phosphonate connected to the ring with a 0 to 3 carbon linker,  
5  
6 -SO<sub>3</sub>H, -CH<sub>2</sub>SO<sub>3</sub>H, -CH<sub>2</sub>CH<sub>2</sub>SO<sub>3</sub>H, -CH<sub>2</sub>CHNH<sub>2</sub>SO<sub>3</sub>H, -CH<sub>2</sub>CH[NHCOCH<sub>2</sub>]<sub>2</sub>SO<sub>3</sub>H,  
7 -CH<sub>2</sub>CH[NHCO(CH<sub>2</sub>)<sub>15</sub>CH<sub>3</sub>]SO<sub>3</sub>H, -CH<sub>2</sub>CH[NH-FMOC]SO<sub>3</sub>H, -CH<sub>2</sub>  
8 CH[NH-tBOC]SO<sub>3</sub>H, or a sulfate or sulfite connected to the ring with a 0 to 3 carbon  
9 linker,  
10  
11 or acts as the functional equivalent of CH<sub>2</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H of T3 in the molecular  
12 recognition domain when bound to a TR, wherein said R<sub>1</sub> can be optionally  
13 substituted with an amine,

14  
15 wherein R<sub>2</sub> is

16 H, halogen, CF<sub>3</sub>, OH, NH<sub>2</sub>, SH, CH<sub>3</sub>, -Et,

17 or acts as the functional equivalent of H in the molecular recognition domain when  
18 bound to a TR,

19  
20 wherein R<sub>3</sub> is

21 -H, halogen, -CF<sub>3</sub>, -OH, -NH<sub>2</sub>, -N<sub>3</sub>, -SH, -CH<sub>3</sub>, -Et,

22 or acts as the functional equivalent of I in the molecular recognition domain when  
23 bound to a TR,

1 wherein  $R_5$  is

2 -H, halogen,  $-CF_3$ ,  $-OH$ ,  $-NH_2$ ,  $-N_3$ ,  $-SH$ ,  $-CH_3$ ,  $-Et$ , or acts as the functional  
3 equivalent of I in the molecular recognition domain when bound to a TR, and  $R_3$  can  
4 be identical to  $R_5$ ,

5

6 wherein  $R_6$  is

7 -H, halogen,  $-CF_3$ ,  $-OH$ ,  $-NH_2$ ,  $-SH$ ,  $-CH_3$ , or acts as the functional equivalent of H  
8 in the molecular recognition domain when bound to a TR, and  $R_2$  can be identical to  
9  $R_6$ ,

10

11 wherein  $R_2'$  is

12 -H, halogen,  $-CF_3$ ,  $-OH$ ,  $-NH_2$ ,  $-N_3$ ,  $-SH$ ,  $-CH_3$ ,  $-Et$ , or acts as the functional  
13 equivalent of H in the molecular recognition domain when bound to a TR,

14

15 wherein  $R_3'$  is any hydrophobic group, including

16 halogen,  $-CF_3$ ,  $-SH$ , alkyl, aryl, 5- or 6-membered heterocyclic, cyano, or acts as the  
17 functional equivalent of I in the molecular recognition domain when bound to a TR,

18

19 wherein  $R_4'$  is

20 -H, halogen,  $-CF_3$ ,  $-OH$ ,  $-NH_2$ ,  $NH_3$ ,  $-N(CH_3)_3$ , carboxylate, phosphonate, phosphate  
21 or sulfate,  $-SH$ ,  $-CH_3$ ,  $-Et$ , or alkyl, aryl or 5- or 6-membered heterocyclic aromatic  
22 attached through urea or carbamate linkages to O or N or S at the  $R_4'$  position, or

1 acts as the functional equivalent of OH in the molecular recognition domain when  
2 bound to a TR,  
3  
4 wherein  $R_5'$  is  
5 -H, -OH, -NH<sub>2</sub>, -N(CH<sub>3</sub>)<sub>2</sub>, -SH, -NH<sub>3</sub>, -N(CH<sub>3</sub>)<sub>3</sub>, carboxylate, phosphonate, phosphate,  
6 sulfate, branched or straight chain alkyl having 1 to 9 carbons, substituted or  
7 unsubstituted aryl, wherein said substituted aryl is substituted with halogen or 1 to 5  
8 carbon alkyl and wherein said aryl is optionally connected to the ring by a -CH<sub>2</sub>-,  
9 aromatic heterocycle having 5 to 6 atoms, wherein said heterocycle may be substituted  
10 with one or more groups selected from -OH, -NH<sub>2</sub>, -SH, -NH<sub>3</sub>, -N(CH<sub>3</sub>)<sub>3</sub>,  
11 carboxylate, phosphonate, phosphate or sulfate, heteroalkyl, arylalkyl, heteroaryl  
12 alkyl, polyaromatic, or polyheteroaromatic, wherein said  $R_5'$  may be substituted with  
13 polar or charged groups,

14  
15 wherein  $R_6'$  is

16 -H, halogen, -CF<sub>3</sub>, -OH, -NH<sub>2</sub>, -SH, -CH<sub>3</sub>, -Et, or acts as the functional equivalent of  
17 H in the molecular recognition domain when bound to a TR,

18  
19 wherein X is

20 O, S, SO<sub>2</sub>, NH, NR<sub>7</sub>, CH<sub>2</sub>, CHR<sub>7</sub>, CR<sub>7</sub>R<sub>7</sub>, wherein R<sub>7</sub> is alkyl, aryl or 5- or  
21 6-membered heterocyclic aromatic,

22  
23 and wherein said TR LBD ligand has an apparent K<sub>d</sub> for binding TR LBD of 1 μM or less.



11. The method of claim 10, wherein

$R_1$  is carboxylate, phosphonate, phosphate or sulfite and is connected to the ring with a 0 to 3 carbon linker,

$R_2$  is H,

$R_3$  is -I, -Br, or -CH<sub>3</sub>,

$R_5$  is -I, -Br, or -CH<sub>3</sub>,

$R_6$  is H,

$R_2'$  is H,

$R_3'$  is -I, -Br, -CH<sub>3</sub>, -iPr, -phenyl, benzyl, or 5- or 6-membered ring heterocycles,

$R_4'$  is -OH, -NH<sub>2</sub>, and -SH,

$R_5'$  is -H, -OH, -NH<sub>2</sub>, -N(CH<sub>3</sub>)<sub>2</sub> -SH -NH<sub>3</sub>, -N(CH<sub>3</sub>)<sub>3</sub>, carboxylate, phosphonate, phosphate, sulfate, branched or straight chain alkyl having 1 to 9 carbons, substituted or unsubstituted aryl, wherein said substituted aryl is substituted with halogen or 1 to 5 carbon alkyl and wherein said aryl is optionally connected to the ring by a -CH<sub>2</sub>-, aromatic heterocycle having 5 to 6 atoms, wherein said heterocycle may be substituted with one or more groups selected from -OH, -NH<sub>2</sub>, -SH, -NH<sub>3</sub>, -N(CH<sub>3</sub>)<sub>3</sub>, carboxylate, phosphonate, phosphate or sulfate, heteroalkyl, arylalkyl, heteroaryl alkyl, polyaromatic, or polyheteroaromatic, wherein said  $R_5'$  may be substituted with polar or charged groups, and

$R_6'$  is H.

1           12.     The method of claim 8, wherein said compound fits spatially and preferentially  
2 into TR LBD isoform  $\alpha$  (TR- $\alpha$ ).

3  
4           13.     The method of claim 12, wherein said compound comprises an anionic group  
5 that interacts with the side chain oxygen or carbon of a serine residue corresponding to  
6 Ser277 of human TR- $\alpha$ , and wherein the anionic group is 1.7-4.0Å from the side chain atom.

7  
8           14.     The method of claim 8, wherein said compound fits spatially and preferentially  
9 into TR LBD isoform  $\beta$  (TR- $\beta$ ).

10  
11           15.     The method of claim 14, wherein said compound comprises an anionic group  
12 that interacts with the side chain nitrogen of an arginine corresponding to Asn331 of human  
13 TR- $\beta$ , and the anionic group is 1.7-4.0Å from the side chain atom.

14  
15           16.     The method of claim 8, wherein said compound binds to a TR LBD isoform  
16 with greater affinity than thyronine or triiodothyronine.

17  
18           17.     A method for identifying a thyroid hormone receptor (TR) agonist or  
19 antagonist ligand, said method comprising the steps of:  
20                   providing the atomic coordinates of a TR ligand binding domain (TR LBD) to  
21 a computerized modeling system;  
22                   modeling ligands which fit spacially into the TR LBD; and

1 identifying in a biological assay for TR activity a ligand which increases or  
2 decreases the activity of said TR, whereby a TR agonist or antagonist is identified.

3  
4 18. A peptide, peptidomimetic or synthetic molecule identified by the method of  
5 any one of claims 8 or 17, with the proviso that said molecule is other than a thyronine or  
6 thyronine-like compound disclosed in a reference cited in Appendix I.

7  
8 19. A method of identifying a compound that selectively modulates the activity of  
9 a thyroid hormone receptor (TR) compared to other nuclear hormone receptors, said method  
10 comprising:

11 modeling compounds which fit spacially into a TR ligand binding domain (TR  
12 LBD) using an atomic structural model of a TR LBD,

13 selecting a compound comprising conformationally constrained structural  
14 features that interact with conformationally constrained residues of a TR LBD,

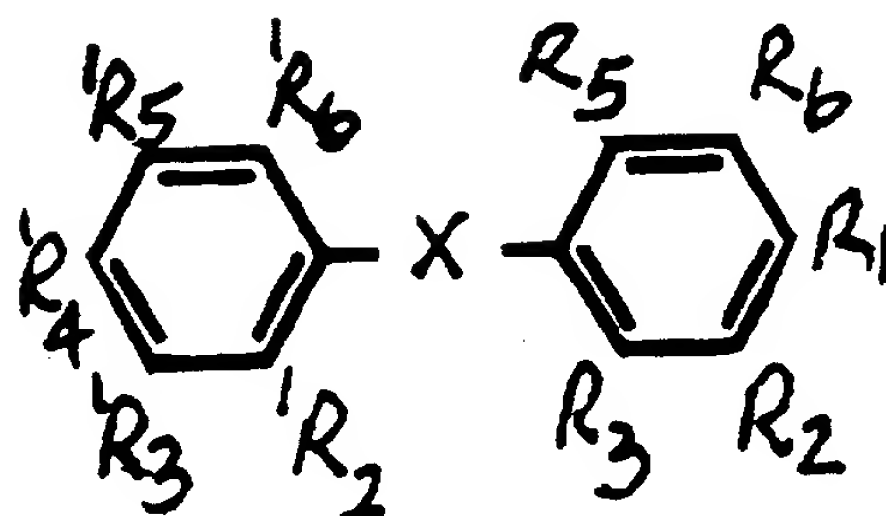
15 identifying in a biological assay for TR activity a compound that selectively  
16 binds to a TR LBD compared to other nuclear receptors, whereby a compound that  
17 selectively modulates a TR is identified.

18

19 20. The method of claim 19, wherein said conformationally constrained residues of  
20 a TR LBD correspond to residues Met259, Leu276, Leu292, His381, Gly290, Ile221, and  
21 Phe401 of human TR- $\alpha$ , and residues Met313, Leu330, Leu346, His435, Gly344, Ile275 and  
22 Phe455 of human TR- $\beta$ .

23

21. The method of claim 19, wherein said compounds are of the formula:



which comprises the following substituents:

(i) an R<sub>1</sub>-substituent comprising an anionic group that interacts with a side chain nitrogen atom of an arginine corresponding to a residue selected from the group consisting of Arg228, Arg262, and Arg266 of human TR- $\alpha$ , and Arg282, Arg316 and Arg320 of human TR- $\beta$ , and wherein the anionic group is 1.7-4.0Å from the nitrogen atom;

(ii) an R<sub>2</sub>-substituent comprising a hydrophobic or hydrophilic group that fits spacially into the TR LBD;

(iii) an R<sub>3</sub>-substituent comprising a hydrophobic or hydrophilic group that interacts with a side chain atom of a serine, alanine or isoleucine corresponding to a residue selected from the group consisting of Ser260, Ala263 and Ile299 of human TR- $\alpha$ , and Ser314, Ala317 and Ile352 of human TR- $\beta$ , and wherein the hydrophobic or hydrophilic group is 1.7-4.0Å from the side chain atom;

(iv) an R<sub>5</sub>-substituent comprising a hydrophobic or hydrophilic group that interacts with a side chain atom of a phenylalanine or isoleucine corresponding to a residue selected from the group consisting of Phe218, Ile221 and Ile222 of human TR- $\alpha$ , and Phe272, Ile275

1 and Ile276 of human TR- $\beta$ , and wherein the hydrophobic or hydrophilic group is 1.7-4.0Å  
2 from the side chain atom;

3 (v) an R6-substituent comprising a hydrophobic or hydrophilic group that fits  
4 spacially into the TR LBD;

5 (vi) an X-substituent comprising a hydrophobic or hydrophilic group that interacts  
6 with a side chain atom of a leucine corresponding to a residue selected from the group  
7 consisting of Leu276 and Leu292 of human TR- $\alpha$ , and Leu 330 and Leu346 of human TR- $\beta$ ,  
8 and wherein the hydrophobic or hydrophilic group is 1.7-4.0Å from the side chain atom;

9 (vii) an R2'-substituent comprising a hydrophobic or hydrophilic group that fits  
10 spacially into the TR LBD;

11 (viii) an R3'-substituent comprising a hydrophobic group that interacts with a side  
12 chain atom of a phenylalanine, glycine or methionine corresponding to a residue selected  
13 from the group consisting of Phe215, Gly290, and Met388 of human TR- $\alpha$ , and Phe269,  
14 Gly344, Met442 of human TR- $\beta$ , and wherein the hydrophobic group is 1.7-4.0Å from the  
15 side chain atom;

16 (ix) an R4'-substituent comprising an hydrogen bond donor or acceptor group that  
17 interacts with a side chain carbon or nitrogen atom of a histidine corresponding to residue  
18 His381 of human TR- $\alpha$ , and His435 of human TR- $\beta$ , and wherein the hydrogen bond donor  
19 or acceptor group is 1.7-4.0Å from the side chain atom;

20 (x) an R5'-substituent comprising a hydrophobic or hydrophilic group that fits  
21 spacially into the TR LBD; and

22 (xi) and R6'-substituent comprising a hydrophobic or hydrophilic group that fits  
23 spacially into the TR LBD.



22. The method of claim 19, wherein said compound comprises:

(i) a cyclic carbon atom that interacts with a carbon and oxygen atom of a methionine residue corresponding to Met259 of human TR- $\alpha$ , and Met313 of human TR- $\beta$ , wherein the cyclic carbon is about 3.0 to 4.0Å from the carbon and oxygen atom of the methionine;

(ii) a cyclic carbon atom that interacts with a carbon atom of a leucine residue corresponding to Leu276 of human TR- $\alpha$ , and Leu330 of human TR- $\beta$ , wherein the cyclic carbon is about 3.0 to 4.0Å from the carbon atom of the leucine;

(iii) a cyclic carbon atom that interacts with a carbon atom of a leucine residue corresponding to Leu292 of human TR- $\alpha$ , and Leu346 of human TR- $\beta$ , wherein the cyclic carbon is about 3.0 to 4.0Å from the carbon atom of the leucine;

(iv) a R3-substituent comprising an atom that interacts with a carbon atom of an isoleucine residue corresponding to Ile221 of human TR- $\alpha$ , and Ile275 of human TR- $\beta$ , wherein the R3-substituent atom is about 3.0 to 4.0Å from the carbon atom of the isoleucine;

(v) a R3'-substituent comprising an atom that interacts with an oxygen atom of a glycine residue corresponding to Gly290 of human TR- $\alpha$ , and Gly344 of human TR- $\beta$ , wherein the R3'-substituent atom is about 3.0 to 4.0Å from the carbon atom of the glycine;

and

(vi) a R4'-substituent comprising an atom selected from the group consisting of oxygen and carbon that interacts with (a) a carbon and nitrogen atom of a histidine residue corresponding to His381 of human TR- $\alpha$ , and His435 of human TR- $\beta$ , wherein the R4'-substituent atom is about 2.0 to 4.0Å from the carbon atom of the histidine; and (b) a carbon atom of a phenylalanine residue corresponding to Phe401 of human TR- $\alpha$ , and human

1 Phe455 of TR- $\beta$ , wherein said atom is about 3.0 to 4.0Å from the carbon atom of the  
2 phenylalanine.

3  
4 23. The method according to claim 21,

5 wherein  $R_1$  is

6 -O-CH<sub>2</sub>CO<sub>2</sub>H, -NHCH<sub>2</sub>CO<sub>2</sub>H,

7 -CO<sub>2</sub>H, -CH<sub>2</sub>CO<sub>2</sub>H, -CH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H, -CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H,

8 -CH<sub>2</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H, -CH<sub>2</sub>CH[NHCOCH $\phi_2$ ]CO<sub>2</sub>H, -CH<sub>2</sub>CH[NHCO(CH<sub>2</sub>)<sub>15</sub>CH<sub>3</sub>

9 ]CO<sub>2</sub>H, -CH<sub>2</sub>CH[NH-FMOC]CO<sub>2</sub>H, -CH<sub>2</sub>CH[NH-tBOC]CO<sub>2</sub>H, or a carboxylate

10 connected to the ring with a 0 to 3 carbon linker,

11  
12 -PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>CH<sub>2</sub>PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>CHNH<sub>2</sub>PO<sub>3</sub>H<sub>2</sub>,

13 -CH<sub>2</sub>CH[NHCOCH $\phi_2$ ]PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>CH[NHCO(CH<sub>2</sub>)<sub>15</sub>CH<sub>3</sub>]PO<sub>3</sub>H<sub>2</sub>,

14 -CH<sub>2</sub>CH[NH-FMOC]PO<sub>3</sub>H<sub>2</sub>, -CH<sub>2</sub>CH[NH-tBOC]PO<sub>3</sub>H<sub>2</sub>, or a phosphate or

15 phosphonate connected to the ring with a 0 to 3 carbon linker,

16  
17 -SO<sub>3</sub>H, -CH<sub>2</sub>SO<sub>3</sub>H, -CH<sub>2</sub>CH<sub>2</sub>SO<sub>3</sub>H, -CH<sub>2</sub>CHNH<sub>2</sub>SO<sub>3</sub>H, -CH<sub>2</sub>CH[NHCOCH $\phi_2$ ]SO<sub>3</sub>H,

18 -CH<sub>2</sub>CH[NHCO(CH<sub>2</sub>)<sub>15</sub>CH<sub>3</sub>]SO<sub>3</sub>H, -CH<sub>2</sub>CH[NH-FMOC]SO<sub>3</sub>H, -CH<sub>2</sub>

19 CH[NH-tBOC]SO<sub>3</sub>H, or a sulfate or sulfite connected to the ring with a 0 to 3 carbon

20 linker,

21

1 or acts as the functional equivalent of  $\text{CH}_2\text{CH}(\text{NH}_2)\text{CO}_2\text{H}$  of T3 in the molecular  
2 recognition domain when bound to a TR, wherein said  $\text{R}_1$  can be optionally  
3 substituted with an amine,

4  
5 wherein  $\text{R}_2$  is

6 H, halogen,  $\text{CF}_3$ , OH,  $\text{NH}_2$ , SH,  $\text{CH}_3$ , -Et,

7 or acts as the functional equivalent of H in the molecular recognition domain when  
8 bound to a TR,

9  
10 wherein  $\text{R}_3$  is

11 -H, halogen,  $-\text{CF}_3$ , -OH,  $-\text{NH}_2$ ,  $-\text{N}_3$ , -SH,  $-\text{CH}_3$ , -Et,

12 or acts as the functional equivalent of I in the molecular recognition domain when  
13 bound to a TR,

14  
15 wherein  $\text{R}_5$  is

16 -H, halogen,  $-\text{CF}_3$ , -OH,  $-\text{NH}_2$ ,  $-\text{N}_3$ , -SH,  $-\text{CH}_3$ , -Et, or acts as the functional

17 equivalent of I in the molecular recognition domain when bound to a TR, and  $\text{R}_3$  can

18 be identical to  $\text{R}_5$ ,

19  
20 wherein  $\text{R}_6$  is

21 -H, halogen,  $-\text{CF}_3$ , -OH,  $-\text{NH}_2$ , -SH,  $-\text{CH}_3$ , or acts as the functional equivalent of H

22 in the molecular recognition domain when bound to a TR, and  $\text{R}_2$  can be identical to

23  $\text{R}_6$ ,

1 wherein  $R_2'$  is

2 -H, halogen,  $-CF_3$ ,  $-OH$ ,  $-NH_2$ ,  $-N_3$ ,  $-SH$ ,  $-CH_3$ ,  $-Et$ , or acts as the functional  
3 equivalent of H in the molecular recognition domain when bound to a TR,

4  
5 wherein  $R_3'$  is any hydrophobic group, including

6 halogen,  $-CF_3$ ,  $-SH$ , alkyl, aryl, 5- or 6-membered heterocycle, cyano, or acts as the  
7 functional equivalent of I in the molecular recognition domain when bound to a TR,

8  
9 wherein  $R_4'$  is

10 -H, halogen,  $-CF_3$ ,  $-OH$ ,  $-NH_2$ ,  $NH_3$ ,  $-N(CH_3)_3$ , carboxylate, phosphonate, phosphate  
11 or sulfate,  $-SH$ ,  $-CH_3$ ,  $-Et$ , or alkyl, aryl or 5- or 6-membered heterocyclic aromatic  
12 attached through urea or carbamate linkages to O or N or S at the  $R_4'$  position, or  
13 acts as the functional equivalent of OH in the molecular recognition domain when  
14 bound to a TR,

15  
16 wherein  $R_5'$  is

17 -H,  $-OH$ ,  $-NH_2$ ,  $-N(CH_3)_2$ ,  $-SH$ ,  $-NH_3$ ,  $-N(CH_3)_3$ , carboxylate, phosphonate, phosphate,  
18 sulfate, branched or straight chain alkyl having 1 to 9 carbons, substituted or  
19 unsubstituted aryl, wherein said substituted aryl is substituted with halogen or 1 to 5  
20 carbon alkyl and wherein said aryl is optionally connected to the ring by a  $-CH_2-$ ,  
21 aromatic heterocycle having 5 to 6 atoms, wherein said heterocycle may be substituted  
22 with one or more groups selected from  $-OH$ ,  $-NH_2$ ,  $-SH$ ,  $-NH_3$ ,  $-N(CH_3)_3$ ,  
23 carboxylate, phosphonate, phosphate or sulfate, heteroalkyl, arylalkyl, heteroaryl

1 alkyl, polyaromatic, or polyheteroaromatic, wherein said  $R_5$  may be substituted with  
2 polar or charged groups,

3  
4 wherein  $R_6$  is

5 -H, halogen,  $-CF_3$ ,  $-OH$ ,  $-NH_2$ ,  $-SH$ ,  $-CH_3$ ,  $-Et$ , or acts as the functional equivalent of  
6 H in the molecular recognition domain when bound to a TR,

7  
8 wherein X is

9 O, S,  $SO_2$ , NH,  $NR_7$ ,  $CH_2$ ,  $CHR_7$ ,  $CR_7R_7$ , wherein  $R_7$  is alkyl, aryl or 5- or  
10 6-membered heterocyclic aromatic,

11  
12 and wherein said TR LBD ligand has an apparent  $K_d$  for binding TR LBD of 1  $\mu M$  or less.  
13

14 24. The method of claim 23, wherein

15  $R_1$  is carboxylate, phosphonate, phosphate or sulfite and is connected to the  
16 ring with a 0 to 3 carbon linker,

17  $R_2$  is H,

18  $R_3$  is -I, -Br, or  $-CH_3$ ,

19  $R_5$  is -I, -Br, or  $-CH_3$ ,

20  $R_6$  is H,

21  $R_2'$  is H,

22  $R_3'$  is -I, -Br,  $-CH_3$ , -iPr, -phenyl, benzyl, or 5- or 6-membered ring

23 heterocycles,



1  $R_4'$  is -OH, -NH<sub>2</sub>, and -SH,

2  $R_5'$  is -H, -OH, -NH<sub>2</sub>, -N(CH<sub>3</sub>)<sub>2</sub> -SH -NH<sub>3</sub>, -N(CH<sub>3</sub>)<sub>3</sub>, carboxylate,

3 phosphonate, phosphate, sulfate, branched or straight chain alkyl having 1 to 9

4 carbons, substituted or unsubstituted aryl, wherein said substituted aryl is substituted

5 with halogen or 1 to 5 carbon alkyl and wherein said aryl is optionally connected to

6 the ring by a -CH<sub>2</sub>-, aromatic heterocycle having 5 to 6 atoms, wherein said

7 heterocycle may be substituted with one or more groups selected from -OH, -NH<sub>2</sub>, -

8 SH, -NH<sub>3</sub>, -N(CH<sub>3</sub>)<sub>3</sub>, carboxylate, phosphonate, phosphate or sulfate, heteroalkyl,

9 arylalkyl, heteroaryl alkyl, polyaromatic, or polyheteroaromatic, wherein said  $R_5'$

10 may be substituted with polar or charged groups, and

11  $R_6'$  is H.

12  
13 25. The method of claim 19, wherein said compound fits spatially and  
14 preferentially into TR LBD isoform  $\alpha$  (TR- $\alpha$ ).

15  
16 26. The method of claim 25, wherein said compound comprises an anionic group  
17 that interacts with the side chain oxygen or carbon of a serine residue corresponding to  
18 Ser277 of human TR- $\alpha$ , and wherein the anionic group is 1.7-4.0Å from the side chain atom.

19  
20 27. The method of claim 19, wherein said compound fits spatially and  
21 preferentially into TR LBD isoform  $\beta$  (TR- $\beta$ ).

1           28.    The method of claim 27, wherein said compound comprises an anionic group  
2   that interacts with the side chain nitrogen of an arginine corresponding to Asn331 of human  
3   TR- $\beta$ , and the anionic group is 1.7-4.0Å from the side chain atom.

4  
5           29.    The method of claim 19, wherein said compound binds to a TR LBD isoform  
6   with greater affinity than thyronine or triiodothyronine.

7  
8           30.    The method of claim 1, wherein said compound comprises a cyclic carbon  
9   atom that interacts with a carbon and oxygen atom of a methionine residue corresponding to  
10   Met259 of human TR- $\alpha$ , and Met313 of human TR- $\beta$ , wherein the cyclic carbon is about 3.0  
11   to 4.0Å from the carbon and oxygen atom of the methionine.

12  
13           31.    The method of claim 30, wherein said cyclic carbon is inner ring carbon C11.

14  
15           32.    The method of claim 1, wherein said compound comprises a cyclic carbon  
16   atom that interacts with a carbon atom of a leucine residue corresponding to Leu276 of  
17   human TR- $\alpha$ , and Leu330 of human TR- $\beta$ , wherein the cyclic carbon is about 3.0 to 4.0Å  
18   from the carbon atom of the leucine.

19  
20           33.    The method of claim 32, wherein said cyclic carbon is selected from the group  
21   consisting of inner ring carbons C7 and C9.

1           34.    The method of claim 1, wherein said compound comprises a cyclic carbon  
2 atom that interacts with a carbon atom of a leucine residue corresponding to Leu292 of  
3 human TR- $\alpha$ , and Leu346 of human TR- $\beta$ , wherein the cyclic carbon is about 3.0 to 4.0Å  
4 from the carbon atom of the leucine.

5  
6           35.    The method of claim 34, wherein said cyclic carbon is selected from the group  
7 consisting of outer ring carbons C6 and C8.

8  
9           36.    The method of claim 1, wherein said R3-substituent comprises an atom that  
10 interacts with a carbon atom of an isoleucine residue corresponding to Ile221 of human TR-  
11  $\alpha$ , and Ile275 of human TR- $\beta$ , wherein the R3-substituent atom is about 3.0 to 4.0Å from the  
12 carbon atom of the isoleucine.

13  
14           37.    The method of claim 1, wherein said R3'-substituent comprises an atom that  
15 interacts with an oxygen atom of a glycine residue corresponding to Gly290 of human TR- $\alpha$ ,  
16 and Gly344 of human TR- $\beta$ , wherein the R3'-substituent atom is about 3.0 to 4.0Å from the  
17 carbon atom of the glycine.

18  
19           38.    The method of claim 1, wherein said R4'-substituent comprises an atom  
20 selected from the group consisting of oxygen and carbon that interacts with a carbon and  
21 nitrogen atom of a histidine residue corresponding to His381 of human TR- $\alpha$ , and His435 of  
22 human TR- $\beta$ , wherein the R4'-substituent atom is about 2.0 to 4.0Å from the carbon atom of  
23 the histidine.

1           39.     The method of claim 1, wherein said R4'-substituent comprises an oxygen  
2 atom that interacts with a carbon atom of a phenylalanine residue corresponding to Phe401 of  
3 human TR- $\alpha$ , and human Phe455 of TR- $\beta$ , wherein said atom is about 3.0 to 4.0Å from the  
4 carbon atom of the phenylalanine.

5  
6           40.     A method for identifying a thyroid hormone receptor (TR) agonist or  
7 antagonist ligand that selectively modulates the activity of a TR compared to other nuclear  
8 receptors, said method comprising the steps of:

9                 providing the atomic coordinates of a TR ligand binding domain (TR LBD) to  
10 a computerized modeling system;

11                 modeling ligands which fit spacially into the TR LBD and which interact with  
12 conformationally constrained residues of a TR LBD conserved among TR isoforms; and

13                 identifying in a biological assay for TR activity a ligand which selectively  
14 binds to said TR and increases or decreases the activity of said TR, whereby a TR agonist or  
15 antagonist that selectively modulates the activity of a TR is identified.

16  
17           41.     A peptide, peptidomimetic or synthetic molecule identified by the method of any  
18 one of claims 19 or 40, with the proviso that said molecule is other than a thyronine or  
19 thyronine-like compound disclosed in a reference cited in Appendix I.

20  
21           42.     A machine-readable data storage medium, comprising a data storage material  
22 encoded with machine readable data which, when using a machine programmed with  
23 instructions for using said data, is capable of displaying a graphical three-dimensional

1 representation of a molecule or molecular complex for a thyroid hormone ligand binding  
2 pocket comprising structure coordinates of TR- $\alpha$  amino acids corresponding to human TR- $\alpha$   
3 amino acids Met259, Leu276, and Ile221, or a homologue of said molecule or molecular  
4 complex, wherein said homologue comprises a binding pocket that has a root mean square  
5 deviation from the backbone atoms of said amino acids of not more than 1.5Å.

6  
7 43. A machine-readable data storage medium, comprising a data storage material  
8 encoded with machine readable data which, when using a machine programmed with  
9 instructions for using said data, is capable of displaying a graphical three-dimensional  
10 representation of a molecule or molecular complex for a thyroid hormone ligand binding  
11 pocket comprising structure coordinates of TR- $\alpha$  amino acids corresponding to human TR- $\alpha$   
12 amino acids Leu292, His381, Gly290 and Phe401, or a homologue of said molecule or  
13 molecular complex, wherein said homologue comprises a binding pocket that has a root mean  
14 square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

15  
16 44. The machine-readable storage medium according to any one of claims 42 or  
17 43, wherein said binding pocket comprises structure coordinates of TR- $\alpha$  amino acids  
18 corresponding to human TR- $\alpha$  amino acids Met259, Leu276, Leu292, His381, Gly290,  
19 Ile221 and Phe401.

20  
21 45. The machine-readable storage medium according to claim 44, wherein said  
22 binding pocket comprises structure coordinates of TR- $\alpha$  amino acids corresponding to human  
23 TR- $\alpha$  amino acids Arg228, Arg262 and Arg266.



1           46.     The machine-readable storage medium according to claim 44, wherein said  
2 binding pocket comprises structure coordinates of TR- $\alpha$  amino acids corresponding to human  
3 TR- $\alpha$  amino acids Ser260, Ala263 and Ile299.

4  
5           47.     The machine-readable storage medium according to claim 44, wherein said  
6 binding pocket comprises structure coordinates of TR- $\alpha$  amino acids corresponding to human  
7 TR- $\alpha$  amino acids Phe218, Ile221 and Ile222.

8  
9           48.     The machine-readable storage medium according to claim 44, wherein said  
10 binding pocket comprises structure coordinates of TR- $\alpha$  amino acids corresponding to human  
11 TR- $\alpha$  amino acids Phe215, Gly290 and Met388.

12  
13           49.     The machine-readable storage medium according to claim 44, wherein said  
14 binding pocket comprises structure coordinates of a TR- $\alpha$  amino acid corresponding to  
15 human TR- $\alpha$  amino acid Ser277.

16  
17           50.     A machine-readable data storage medium, comprising a data storage material  
18 encoded with machine readable data which, when using a machine programmed with  
19 instructions for using said data, is capable of displaying a graphical three-dimensional  
20 representation of a molecule or molecular complex for a thyroid hormone ligand binding  
21 pocket comprising structure coordinates of TR- $\beta$  amino acids corresponding to human TR- $\beta$   
22 amino acids Met313, Leu330, and Ile275, or a homologue of said molecule or molecular

1 complex, wherein said homologue comprises a binding pocket that has a root mean square  
2 deviation from the backbone atoms of said amino acids of not more than 1.5Å.

3  
4 51. A machine-readable data storage medium, comprising a data storage material  
5 encoded with machine readable data which, when using a machine programmed with  
6 instructions for using said data, is capable of displaying a graphical three-dimensional  
7 representation of a molecule or molecular complex for a thyroid hormone ligand binding  
8 pocket comprising structure coordinates of TR- $\beta$  amino acids corresponding to human TR- $\beta$   
9 amino acids Leu346, His435, Gly344, and Phe455, or a homologue of said molecule or  
10 molecular complex, wherein said homologue comprises a binding pocket that has a root mean  
11 square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

12  
13 52. The machine-readable data storage medium according to any one of claims 50  
14 or 51, wherein said binding pocket comprises structure coordinates of TR- $\beta$  amino acids  
15 corresponding to human TR- $\beta$  amino acids Met313, Leu330, Leu346, His435, Gly344,  
16 Ile275 and Phe455.

17  
18 53. The machine-readable data storage medium according to claim 52, wherein  
19 said binding pocket comprises structure coordinates of TR- $\beta$  amino acids corresponding to  
20 human TR- $\beta$  amino acids Arg282, Arg316 and Arg320.

1           54.    The machine-readable data storage medium according to claim 52, wherein  
2   said binding pocket comprises structure coordinates of TR- $\beta$  amino acids corresponding to  
3   human TR- $\beta$  amino acids Ser314, Ala317 and Ile352.

4  
5           55.    The machine-readable data storage medium according to claim 52, wherein  
6   said binding pocket comprises structure coordinates of TR- $\beta$  amino acids corresponding to  
7   human TR- $\beta$  amino acids Phe272, Ile275 and Ile276.

8  
9           56.    The machine-readable data storage medium according to claim 52, wherein  
10   said binding pocket further comprises structure coordinates of TR- $\beta$  amino acids  
11   corresponding to human TR- $\beta$  amino acids Phe269, Gly344 and Met442.

12  
13           57.    The machine-readable data storage medium according to claim 52, wherein  
14   said binding pocket comprises structure coordinates of a TR- $\beta$  amino acid corresponding to  
15   human TR- $\beta$  amino acid Asn331.

16  
17           58.    The machine-readable data storage medium according to claim 52, wherein  
18   said molecule or molecular complex is defined by the set of structure coordinates selected  
19   from the group consisting coordinates depicted in Appendix 3, 4, 5 and 6, or a homologue of  
20   said molecule or molecular complex, said homologue having a root mean square deviation  
21   from the backbone atoms of said amino acids of not more than 1.5Å.

1           59.    The machine-readable data storage medium according to claim 52, wherein  
2   said molecule or molecular complex is defined by the set of structure coordinates selected  
3   from the group consisting coordinates depicted in Appendix 7 and 8, or a homologue of said  
4   molecule or molecular complex, said homologue having a root mean square deviation from  
5   the backbone atoms of said amino acids of not more than 1.5Å.

6  
7           60.    A machine-readable data storage medium comprising a data storage material  
8   encoded with a first set of machine readable data which, when combined with a second set of  
9   machine readable data, using a machine programmed with instructions for using said first set  
10   of data and said second set of data, can determine at least a portion of the structure  
11   coordinates corresponding to the second set of machine readable data, wherein: said first set  
12   of data comprises a Fourier transform of at least a portion of the structural coordinates  
13   selected from the group consisting of coordinates depicted in Appendix 3, 4, 5, 6, 7 and 8;  
14   and said second set of data comprises an X-ray diffraction pattern of a molecule or molecular  
15   complex.

## APPENDIX 1

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## APPENDIX 2

Table 8

Dimit Atom	Amino Acid in full length $\alpha$	Amino Acid Atom	<u>Distance</u> A
C16	215-PHE	CD1	3.98
C16	215-PHE	CE1	3.86
C19	218-PHE	O	3.69
C16	218-PHE	CB	3.89
C18	218-PHE	CB	3.92
C19	218-PHE	CB	4.13
C18	218-PHE	CD2	3.77
C16	219-THR	CG2	3.68
C19	221-ILE	CG1	4.11
C6	222-ILE	CD1	4.18
C8	222-ILE	CD1	3.72
C10	222-ILE	CD1	3.53
C12	222-ILE	CD1	3.85
O1	222-ILE	CD1	4.13
C13	225-ALA	C8	3.64
O4	225-ALA	C8	4.02
O4	228-ARG	CZ	3.96
C17	228-ARG	NH2	3.36
O3	228-ARG	NH2	3.58
O4	228-ARG	NH2	2.86
C10	256-MET	SD	3.70
C12	256-MET	SD	3.89
C10	256-MET	CE	3.88
C12	256-MET	CE	3.83
C11	259-MET	C	4.03
C11	259-MET	O	3.66
C15	259-MET	O	3.42
N1	259-MET	O	3.71
C1	259-MET	C8	4.20
C11	259-MET	C8	3.87
C13	259-MET	C8	4.09
C15	262-ARG	C8	4.03
C17	262-ARG	C8	3.58
O3	262-ARG	C8	3.62
O4	262-ARG	C8	3.85
C17	262-ARG	CD	4.10
O4	262-ARG	CD	3.61
N1	263-ALA	N	3.71
C17	263-ALA	CA	3.69
N1	263-ALA	CB	3.46
O3	266-ARG	NH1	3.93
N1	275-THR	O	3.62
N1	276-LEU	CA	3.51
N1	276-LEU	C	3.92
C5	276-LEU	CD1	4.05
C19	276-LEU	CD1	4.04
C7	276-LEU	CD2	4.09
C9	276-LEU	CD2	3.95
C11	276-LEU	CD2	4.13
N1	276-LEU	CD2	4.17
C13	277-SER	N	4.14
C15	277-SER	N	3.79

	Dimit Atom	Amino Acid in full length $\alpha$	Atom	Distance A
1				
2				
3	C17	277-SER	N	3.69
4	N1	277-SER	N	3.30
5	O3	277-SER	N	3.19
6	C17	277-SER	CA	3.92
7	O3	277-SER	CA	3.35
8	C13	277-SER	OG	3.92
9	C7	287-LEU	CD2	3.90
10	C18	290-GLY	C	4.04
11	C18	290-GLY	O	3.54
12	C18	291-GLY	CA	4.04
13	C18	292-LEU	N	4.20
14	C2	292-LEU	CG	4.18
15	C4	292-LEU	CG	3.86
16	C6	292-LEU	CG	4.01
17	C2	292-LEU	CD1	3.88
18	C4	292-LEU	CD1	4.02
19	O2	292-LEU	CD1	4.07
20	C4	292-LEU	CD2	4.05
21	C6	292-LEU	CD2	3.72
22	C8	292-LEU	CD2	3.69
23	C10	292-LEU	CD2	3.98
24	O1	292-LEU	CD2	4.16
25	C20	299-ILE	CD1	3.87
26	C8	381-HIS	CD2	3.90
27	C10	381-HIS	CD2	3.84
28	O1	381-HIS	GO2	3.40
29	O1	381-HIS	CE1	3.72
30	C8	381-HIS	NE2	3.47
31	C10	381-HIS	NE2	3.51
32	O1	381-HIS	NE2	2.64
33	C6	388-MET	CE	3.90
34	C8	401-PHE	CE1	4.19
35	O1	401-PHE	CE1	3.37
36	C16	401-PHE	CZ	3.97
37	O1	401-PHE	CZ	3.28
38	N1	502-H <sub>2</sub> O	O1	3.35
39	O3	502-H <sub>2</sub> O	O1	2.56
40	O3	503-H <sub>2</sub> O	O1	3.13
41	O4	503-H <sub>2</sub> O	O1	3.72
42	O4	504-H <sub>2</sub> O	O1	2.72

Legend to Table 8. The table lists the interactions with Dimit (DMT). The column headings are as follows:

#1 The atom of Dimit that interacts with the amino acid of the receptor. These are also numbered in figure 32.

#2 The amino acid in the full length rTR $\alpha$  that interacts with the ligand.

#3 The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.

#4 The distance in A between Dimit and the protein atom.



Table 9

Triac Atom	Amino Acid in full length $\alpha$	Amino Acid Atom	Distance A
I1	218-PHE	O	3.52
I1	221-ILE	CD1	4.16
I1	221-ILE	CG1	3.92
I1	222-ILE	CA	4.15
I1	222-ILE	CB	4.03
I1	222-ILE	CG1	3.92
C8	222-ILE	CD1	4.12
C10	222-ILE	CD1	3.77
C12	222-ILE	CD1	3.79
C13	225-ALA	CB	4.17
C3	225-ALA	CB	3.86
C10	256-MET	SD	3.45
C12	256-MET	SD	3.73
C10	256-MET	CE	3.66
C12	256-MET	CE	3.77
I3	256-MET	CE	3.89
C1	259-MET	O	3.93
C11	259-MET	O	3.24
O3	259-MET	O	4.09
C1	259-MET	CB	3.89
C13	259-MET	O	3.74
C14	259-MET	O	3.96
C1	259-MET	CB	3.89
C11	259-MET	CB	3.68
C13	259-MET	CB	4.01
C11	259-MET	CA	4.13
C13	259-MET	CA	4.20
I3	260-SER	CA	4.10
I3	260-SER	OG	4.19
C14	262-ARG	CB	4.07
O4	262-ARG	CB	3.60
O3	263-ALA	N	3.79
C14	263-ALA	N	4.12
O3	263-ALA	CA	3.67
O3	263-ALA	CB	3.49
C11	263-ALA	CB	4.00
C14	266-ARG	CZ	3.89
O3	266-ARG	CZ	4.01
O4	266-ARG	CZ	3.03
C14	266-ARG	NH1	3.25
O3	266-ARG	NH1	3.00
O4	266-ARG	NH1	2.82
C14	266-ARG	NH2	3.48
O3	266-ARG	NH2	4.01
O4	266-ARG	NH2	2.34
O3	275-THR	C	4.02
C14	275-THR	O	4.20
O3	275-THR	O	3.20
O3	278-LEU	CA	3.11
O3	276-LEU	C	3.52
O3	276-LEU	N	4.04
C14	276-LEU	CA	3.98
O3	276-LEU	CA	3.11

	Triac Atom	Amino Acid in full length $\alpha$	Amino Acid Atom	Distance A
1	C14	276-LEU	C	3.98
2	O3	276-LEU	CB	3.95
3	O2	276-LEU	CD1	4.03
4	I1	276-LEU	CD1	4.10
5	C7	276-LEU	CD2	3.84
6	C9	276-LEU	CD2	3.73
7	Cl1	276-LEU	CD2	4.06
8	O2	276-LEU	CD2	4.10
9	O3	276-LEU	CD2	3.91
10	C13	277-SER	N	4.06
11	C14	277-SER	N	3.13
12	O4	277-SER	N	3.28
13	O3	277-SER	N	3.05
14	C14	277-SER	CA	3.76
15	O4	277-SER	CA	3.52
16	C3	277-SER	OG	3.87
17	C13	277-SER	OG	4.02
18	C14	277-SER	OG	4.14
19	I2	290-GLY	O	3.57
20	I2	292-LEU	CG	3.94
21	C4	292-LEU	CG	3.95
22	C6	292-LEU	CG	3.65
23	C8	292-LEU	CG	4.02
24	C2	292-LEU	CD1	4.11
25	C4	292-LEU	CD1	3.85
26	C6	292-LEU	CD1	4.02
27	I2	292-LEU	CD2	3.98
28	C4	292-LEU	CD2	4.11
29	C6	292-LEU	CD2	3.44
30	C8	292-LEU	CD2	3.28
31	C10	292-LEU	CD2	3.88
32	O1	292-LEU	CD2	3.35
33	I3	299-ILE	CD1	3.77
34	C8	381-HIS	CD2	3.87
35	C10	381-HIS	CD2	3.90
36	O1	381-HIS	GO2	3.20
37	O1	381-HIS	CE1	3.82
38	C8	381-HIS	NE2	3.57
39	C10	381-HIS	NE2	3.52
40	O1	381-HIS	NE2	2.64
41	O1	388-MET	CE	4.03
42	O1	401-PHE	CE1	3.86
43	O1	401-PHE	CZ	3.70
44	C13	460-H <sub>2</sub> O	O1	4.00

Legend to Table 9. The table lists the interactions with Triac. The column headings are as follows:  
 #1 The atom of Triac that interacts with the amino acid of the receptor. These are also numbered in figure 32.

#2 The amino acid in the full length rTR $\alpha$  that interacts with the ligand.

#3 The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.

#4 The distance in A between Triac and the protein atom.

Table 10

	IpBR <sub>2</sub> Atom	Amino Acid in full length $\alpha$	Amino Acid Atom	Distance A
3	C16	215-PHE	CD1	4.01
4	C16	215-PHE	CE1	3.78
5	BR1	218-PHE	O	3.24
6	BR1	218-PHE	C	3.98
7	C16	218-PHE	CB	3.81
8	C18	218-PHE	CB	3.92
9	BR1	218-PHE	CB	4.08
10	C18	218-PHE	CD2	3.92
11	C16	219-THR	CG2	3.45
12	BR1	221-ILE	CG1	3.81
13	BR1	221-ILE	CD1	4.07
14	BR1	222-ILE	CB	3.81
15	BR1	222-ILE	CG1	3.97
16	C6	222-ILE	CD1	4.07
17	C8	222-ILE	CD1	3.64
18	C10	222-ILE	CD1	3.50
19	C12	222-ILE	CD1	3.82
20	O1	222-ILE	CD1	4.08
21	C13	225-ALA	CB	3.76
22	O4	225-ALA	CB	4.01
23	O4	228-ARG	CZ	3.92
24	C17	228-ARG	NH2	3.26
25	O3	228-ARG	NH2	3.43
26	O4	228-ARG	NH2	2.79
27	C10	256-MET	SD	3.65
28	C12	256-MET	SD	3.71
29	C10	256-MET	CE	3.90
30	C12	256-MET	CE	3.75
31	BR2	256-MET	CE	4.03
32	C11	259-MET	C	3.98
33	C11	259-MET	O	3.52
34	C15	259-MET	O	3.44
35	N1	259-MET	O	3.76
36	C11	259-MET	CB	3.87
37	N1	262-ARG	C	4.03
38	C15	262-ARG	CB	4.03
39	C17	262-ARG	CB	3.56
40	O3	262-ARG	CB	3.55
41	O4	262-ARG	CB	3.91
42	C17	262-ARG	CD	4.09
43	O4	262-ARG	CD	3.71
44	N1	263-ALA	N	3.61
45	N1	263-ALA	CA	3.59
46	N1	263-ALA	CB	3.54
47	O3	266-ARG	NH1	3.93
48	N1	275-THR	O	3.43
49	N1	276-LEU	CA	3.46
50	N1	276-LEU	C	3.83
51	C5	276-LEU	CD1	4.02
52	C7	276-LEU	CD2	4.00
53	C9	276-LEU	CD2	3.81
54	C11	276-LEU	CD2	3.91
55	C13	277-SER	N	3.79

IpBr <sub>2</sub> Atom		Amino Acid in full length $\alpha$	Amino Acid Atom	Distance A
1	C15	277-SER	N	3.63
2	C17	277-SER	N	3.70
3	N1	277-SER	N	3.17
4	O3	277-SER	N	3.37
5	C17	277-SER	CA	3.89
6	O3	277-SER	CA	3.43
7	C13	277-SER	OG	3.66
8	O2	287-LEU	CD1	4.05
9	C18	290-GLY	C	4.04
10	C18	290-GLY	O	3.48
11	C18	291-GLY	CA	4.02
12	C4	292-LEU	CG	3.89
13	C6	292-LEU	CG	4.02
14	C2	292-LEU	CD1	3.79
15	C4	292-LEU	CD1	3.96
16	O2	292-LEU	CD1	3.97
17	C4	292-LEU	CD2	4.07
18	C6	292-LEU	CD2	3.75
19	C8	292-LEU	CD2	3.67
20	C10	292-LEU	CD2	3.92
21	BR2	299-ILE	CD1	3.68
22	C8	381-HIS	CD2	3.92
23	C10	381-HIS	CD2	3.78
24	O1	381-HIS	GD2	3.50
25	O1	381-HIS	CE1	3.62
26	C8	381-HIS	NE2	3.36
27	C10	381-HIS	NE2	3.34
28	O1	381-HIS	NE2	2.62
29	C8	401-PHE	CE1	4.02
30	O1	401-PHE	CE1	3.19
31	C16	401-PHE	CZ	4.03
32	O1	401-PHE	CZ	3.06
33	O3	502-H <sub>2</sub> O	O1	3.40
34	N1	502-H <sub>2</sub> O	O1	3.12
35	O4	503-H <sub>2</sub> O	O1	3.20
36	C17	503-H <sub>2</sub> O	O1	3.04
37	O3	503-H <sub>2</sub> O	O1	2.27
38	C15	504-H <sub>2</sub> O	O1	4.01
39	C17	504-H <sub>2</sub> O	O1	2.99
40	O3	504-H <sub>2</sub> O	O1	3.80
41	O4	504-H <sub>2</sub> O	O1	1.78

Legend to Table 10. The table lists the interactions with IpBr<sub>2</sub>. The column headings are as follows:

- #1 The atom of IpBr<sub>2</sub> that interacts with the amino acid of the receptor. These are also numbered in figure 32.
- #2 The amino acid in the full length rTR $\alpha$  that interacts with the ligand.
- #3 The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.
- #4 The distance in A between IpBr<sub>2</sub> and the protein atom.

Table 11

	T3 Atom	Amino Acid in full length $\alpha$	Amino Acid Atom	Distance A
3	I2	215-PHE	CD1	4.08
4	I1	218-PHE	O	3.19
5	I1	218-PHE	CB	3.99
6	C4	218-PHE	CB	4.04
7	I1	218-PHE	C	3.79
8	I1	218-PHE	CB	3.99
9	I1	221-ILE	CG1	4.01
10	I1	222-ILE	CB	3.95
11	I1	222-ILE	CG1	3.91
12	C8	222-ILE	CD1	3.99
13	C10	222-ILE	CD1	3.57
14	C12	222-ILE	CD1	3.68
15	C13	225-ALA	CB	3.66
16	C3	225-ALA	CB	4.04
17	O4	228-ARG	NH1	3.23
18	O4	228-ARG	CZ	3.45
19	C15	228-ARG	NH2	3.54
20	O3	228-ARG	NH2	3.90
21	O4	228-ARG	NH2	2.86
22	C10	256-MET	SD	3.73
23	C12	256-MET	SD	3.90
24	C10	256-MET	CE	3.97
25	C12	256-MET	CE	3.92
26	I3	256-MET	CE	3.89
27	C11	259-MET	C	3.95
28	C11	259-MET	O	3.59
29	C14	259-MET	O	3.51
30	N1	259-MET	O	3.88
31	C1	259-MET	CB	4.06
32	C11	259-MET	CB	3.77
33	C13	259-MET	CB	3.96
34	C15	262-ARG	CB	3.61
35	C14	262-ARG	CB	4.02
36	O3	262-ARG	CB	3.65
37	O4	262-ARG	CB	3.92
38	O4	262-ARG	CD	3.72
39	N1	263-ALA	N	3.81
40	N1	263-ALA	CA	3.81
41	N1	263-ALA	CB	3.63
42	N1	275-THR	O	3.54
43	N1	276-LEU	CA	3.38
44	N1	276-LEU	C	3.73
45	C5	276-LEU	CD1	4.00
46	C7	276-LEU	CD1	4.05
47	O2	276-LEU	CD1	4.03
48	C7	276-LEU	CD2	3.80
49	C9	276-LEU	CD2	3.70
50	C11	276-LEU	CD2	4.01
51	C14	277-SER	N	3.67
52	C15	277-SER	N	3.62
53	N1	277-SER	N	3.07
54	O3	277-SER	N	3.24
55	C15	277-SER	CA	3.77

	T3 Atom	Amino Acid in full length $\alpha$	Amino Acid Atom	Distance A
1	O3	277-SER	CA	3.34
2	C13	277-SER	OG	3.92
3	I2	290-GLY	O	3.50
4	C4	292-LEU	CG	3.95
5	C8	292-LEU	CG	3.83
6	C2	292-LEU	CD1	4.07
7	C4	292-LEU	CD1	3.99
8	C4	292-LEU	CD2	4.09
9	C6	292-LEU	CD2	3.58
10	C8	292-LEU	CD2	3.50
11	C10	292-LEU	CD2	3.96
12	O1	292-LEU	CD2	3.71
13	I3	299-ILE	CD1	3.74
14	C8	381-HIS	CD2	3.94
15	C10	381-HIS	CD2	3.97
16	O1	381-HIS	CD2	3.39
17	O1	381-HIS	CD1	3.82
18	C8	381-HIS	NE2	3.47
19	C10	381-HIS	NE2	3.55
20	O1	381-HIS	NE2	2.70
21	O1	388-MET	CE	3.88
22	O1	401-PHE	CE1	3.52
23	O1	401-PHE	CZ	3.32
24	C14	502-H2O	O1	4.01
25	C15	502-H2O	O1	3.61
26	O3	502-H2O	O1	2.51
27	C15	503-H2O	O1	3.31
28	O4	503-H <sub>2</sub> O	O1	3.10
29	N1	502-H <sub>2</sub> O	O1	3.27
30	O3	503-H2O	O1	2.81
31	C15	504-H2O	O1	3.92
32	O4	504-H2O	O1	2.73

Legend to Table 11. The table lists the interactions with T3. The column headings are as follows:

- #1 The atom of T3 that interacts with the amino acid of the receptor. These are also numbered in figure 32.
- #2 The amino acid in the full length rTR $\alpha$  that interacts with the ligand.
- #3 The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.
- #4 The distance in A between T3 and the protein atom.



Table 12

	Triac Atom	Amino Acid in full length hTR $\beta$	Amino Acid Atom	Distance A
2				
3				
4	I2	269-PHE	CD1	3.75
5	I2	269-PHE	CE1	3.88
6	I1	272-PHE	C	4.03
7	I1	272-PHE	O	3.54
8	I1	275-ILE	CG1	3.93
9	I1	276-ILE	CG1	4.02
10	C3	279-ALA	CB	3.81
11	C13	279-ALA	CB	3.87
12	C10	310-MET	SD	3.72
13	C12	310-MET	SD	3.78
14	C10	310-MET	CE	4.02
15	C12	310-MET	CE	3.92
16	I3	310-MET	CE	3.93
17	C13	313-MET	CA	3.94
18	C11	313-MET	C	3.72
19	C1	313-MET	O	3.79
20	C11	313-MET	O	3.12
21	C13	313-MET	O	3.55
22	C1	313-MET	CB	4.00
23	C11	313-MET	CB	3.82
24	C13	313-MET	CB	3.76
25	C13	313-MET	CG	3.88
26	O3	316-ARG	CB	3.99
27	O4	317-ALA	CA	4.08
28	O4	317-ALA	CA	4.10
29	C11	317-ALA	CB	3.70
30	I3	317-ALA	CB	4.10
31	O4	317-ALA	CB	4.06
32	O4	320-ARG	NH1	3.58
33	O3	320-ARG	NH2	3.55
34	O4	320-ARG	NH2	4.04
35	O4	329-THR	O	3.55
36	O4	330-LEU	CA	3.42
37	O4	330-LEU	C	3.77
38	C3	330-LEU	CB	4.06
39	C5	330-LEU	CB	4.08
40	C1	330-LEU	CD2	4.07
41	C3	330-LEU	CD2	4.00
42	C5	330-LEU	CD2	3.73
43	C7	330-LEU	CD2	3.51
44	C9	330-LEU	CD2	3.54
45	C11	330-LEU	CD2	3.86
46	C15	331-ASN	N	3.55
47	O3	331-ASN	N	3.74
48	O4	331-ASN	N	3.12
49	O3	331-ASN	CA	4.02
50	I2	344-GLY	O	3.87
51	C6	346-LEU	CD2	3.87
52	C8	346-LEU	CD2	3.84
53	O1	346-LEU	CD2	3.91
54	I3	353-ILE	CD1	3.51
55	C8	435-HIS	CD2	3.93
56	C10	435-HIS	CD2	3.79

Triac Atom	Amino Acid in full length hTR $\beta$	Amino Acid Atom	Distance A
O1	435-HIS	CD2	3.33
O1	435-HIS	CE1	3.81
C8	435-HIS	NE2	3.42
C10	435-HIS	NE2	3.33
O1	435-HIS	NE2	2.67
O1	442-MET	SD	3.96
O1	442-MET	CE	3.72
I2	442-MET	SD	4.01
O1	455-PHE	CE1	3.92
O1	455-PHE	CZ	3.50

Legend to Table 12. The table lists the interactions with Triac. The column headings are as follows:

- #1 The atom of Triac that interacts with the amino acid of the receptor. These are also numbered in figure 32.
- #2 The amino acid in the full length hTR $\beta$  that interacts with the ligand.
- #3 The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.
- #4 The distance in A between Triac and the protein atom.

Table 13

	GC1 Atom	Amino Acid in full length TR $\beta$	Amino Acid Atom	Distance A
2				
3				
4	C16	269-PHE	CE1	3.99
5	C19	272-PHE	O	3.85
6	C16	272-PHE	CB	3.98
7	C16	273-THR	CG2	3.76
8	C19	275-ILE	CG1	3.98
9	C19	276-ILE	CA	3.98
10	C2	276-ILE	CD1	3.88
11	C8	276-ILE	CD1	3.77
12	C10	276-ILE	CD1	3.58
13	C12	276-ILE	CD1	3.62
14	C19	276-ILE	CD1	3.56
15	C1	279-ALA	CB	3.68
16	C3	279-ALA	CB	3.56
17	O5	279-ALA	CB	3.11
18	O4	279-ALA	CB	3.90
19	O3	282-ARG	CZ	3.53
20	C17	282-ARG	NH1	3.87
21	O3	282-ARG	NH1	3.20
22	O4	282-ARG	NH1	3.85
23	C17	282-ARG	NH2	3.63
24	O3	282-ARG	NH2	3.00
25	C10	310-MET	SD	3.86
26	C12	310-MET	SD	3.91
27	C11	313-MET	C	3.85
28	C11	313-MET	O	3.41
29	C15	313-MET	O	3.87
30	C20	313-MET	O	3.99
31	C11	313-MET	CB	3.79
32	C1	313-MET	CG	3.94
33	C11	313-MET	CG	3.91
34	O5	313-MET	CG	3.87
35	O4	313-MET	CG	3.79
36	C20	314-SER	CA	4.00
37	C17	316-ARG	CB	3.95
38	C17	316-ARG	CD	3.80
39	O3	316-ARG	CD	3.83
40	O4	316-ARG	CD	3.51
41	C20	317-ALA	CB	3.93
42	C7	330-LEU	CD2	3.56
43	C9	330-LEU	CD2	3.63
44	C21	330-LEU	CD2	3.90
45	O5	331-ASN	N	3.62
46	C15	331-ASN	N	3.67
47	C18	344-GLY	O	3.60
48	C18	346-LEU	CG	3.89
49	C6	346-LEU	CD2	3.77
50	C8	346-LEU	CD2	3.80
51	C10	435-HIS	CD2	3.89
52	O1	435-HIS	CD2	3.64
53	O1	435-HIS	CE1	3.79
54	C8	435-HIS	NE2	3.44

GC1 Atom	Amino Acid in full length TR $\beta$	Amino Acid Atom	Distance A
C10	435-HIS	NE2	3.33
O1	435-HIS	NE2	2.77
O1	455-PHE	CE1	3.40
O1	455-PHE	CZ	3.22

Legend to Table 13. The table lists the interactions with GC1. The column headings are as follows:

- #1 The atom of GC1 that interacts with the amino acid of the receptor. These are also numbered in figure 32.
- #2 The amino acid in the full length hTR $\beta$  that interacts with the ligand.
- #3 The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.
- #4 The distance in A between GC1 and the protein atom.

Table 14  
Coordination Structure of TR- $\alpha$  and Dimit

Coordination Structure	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>5</sub>	R <sub>6</sub>	R' <sub>2</sub>	R' <sub>3</sub>	R' <sub>4</sub>	R' <sub>5</sub>	R' <sub>6</sub>	X
	-CH <sub>2</sub> - CH(NH <sub>2</sub> )(CO <sub>2</sub> )H	-H	-CH <sub>3</sub>	-CH <sub>3</sub>	-H	-H	-CH(CH <sub>3</sub> ) <sub>2</sub>	-OH	-H	-H	O
AA							215				
SS							H3				
AA			218				218				
SS			H3				H3				
AA							219				
SS							H3				
AA			221								
SS			H3								
AA							222	222	222	222	
SS							H3	H3	H3	H3	
AA	225										
SS	H3										
AA	228										
SS	H3										
AA									256	256	
SS									H5-H6	H5-H6	
AA	259				259						-
SS	H5-H6				H5-H6						
AA	262										
SS	H5-H6										
AA	263										
SS	H5-H6										
AA	266										
SS	loop										
AA	275										
SS	S3										
AA	276		276	276	276						
SS	S3		S3	S3	S3						
AA	277										
SS	loop										
AA							290-291				
SS							loop				
AA						292	292	292	292		292
SS						loop	loop	loop	loop		loop
AA				299							
SS				H8							
AA								381	381		
SS								H11	H11		
AA							388				
SS							H11				
AA							401	401			
SS							H12	H12			
AA	HOH502/HOH503/HOH504										
SS											

AA = Amino Acid

SS = Secondary Structure

Table 15  
Coordination Structure of TR- $\alpha$  and Triac

Coordination Structure	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>5</sub>	R <sub>6</sub>	R' <sub>2</sub>	R' <sub>3</sub>	R' <sub>4</sub>	R' <sub>5</sub>	R' <sub>6</sub>	X
	-CH <sub>2</sub> -COOH	-H	-I	-I	-H	-H	-I	-OH	-H	-H	O
AA			218								
SS	-		H3								
AA			221								
SS			H3								
AA							222	222	222	222	
SS							H3	H3	H3	H3	
AA	225										
SS	H3										
AA				256					256	256	
SS				H5-H6					H5-H6	H5-H6	
AA	259				259						
SS	H5-H6				H5-H6						
AA	262										
SS	H5-H6										
AA	263										
SS	H5-H6										
AA	266										
SS	loop										
AA	275										
SS	S3										
AA	276		276	276	276						
SS	S3		S3	S3	S3						
AA	277										
SS	loop										
AA							290				
SS							loop				
AA						292	292	292	292		292
SS						loop	loop	loop	loop		loop
AA				299							
SS				H8							
AA								381	381		
SS								H11	H11		
AA								388			
SS								H11			
AA							401	401			
SS							H12	H12			

AA = Amino Acid

SS = Secondary Structure



Table 16  
Coordination Structure of TR- $\alpha$  and IpBr2

Coordination Structure	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>5</sub>	R <sub>6</sub>	R' <sub>2</sub>	R' <sub>3</sub>	R' <sub>4</sub>	R' <sub>5</sub>	R' <sub>6</sub>	X
	-CH <sub>2</sub> -CH(NH <sub>2</sub> )(CO <sub>2</sub> )H	-H	-Br	-Br	-H	-H	-CH(CH <sub>3</sub> ) <sub>2</sub>	-OH	-H	-H	O
AA							215				
SS							H3				
AA			218				218				
SS			H3				H3				
AA							219				
SS							H3				
AA			221								
SS			H3								
AA							222	222	222	222	
SS							H3	H3	H3	H3	
AA	225										
SS	H3										
AA	228										
SS	H3										
AA					256				256	256	
SS					H5-H6				H5-H6	H5-H6	
AA	259				259						
SS	H5-H6				H5-H6						
AA	262										
SS	H5-H6										
AA	263										
SS	H5-H6										
AA	266										
SS	loop										
AA	275										
SS	S3										
AA	276		276	276	276						
SS	S3		S3	S3	S3						
AA	277										
SS											
AA							290-291				
SS							loop				
AA						292	292	292	292		292
SS						loop	loop	loop	loop		loop
AA				299							
SS				H8							
AA								381	381		
SS								H11	H11		
AA							401	401			
SS							H12	H12			
AA	HOH502/HOH503/HOH504										
SS											

AA = Amino Acid

SS = Secondary Structure

Table 17  
Coordination Structure of TR- $\alpha$  and Dimit

Coordination Structure	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>5</sub>	R <sub>6</sub>	R' <sub>2</sub>	R' <sub>3</sub>	R' <sub>4</sub>	R' <sub>5</sub>	R' <sub>6</sub>	X
	-CH <sub>2</sub> - CH(NH <sub>2</sub> )(CO <sub>2</sub> )H	-H	-I	-I	-H	-H	-I	-OH	-H	-H	O
AA							215				
SS							H3				
AA			218			218					
SS			H3			H3					
AA			221								
SS			H3								
AA							222	222	222	222	
SS							H3	H3	H3	H3	
AA	225										
SS	H3										
AA	228										
SS	H3										
AA					256				256	256	
SS					H5-H6				H5-H6	H5-H6	
AA	259				259						
SS	H5-H6				H5-H6						
AA	262										
SS	H5-H6										
AA	263										
SS	H5-H6										
AA	275										
SS	S3										
AA	276		276	276	276						
SS	S3		S3	S3	S3						
AA	277										
SS											
AA							290				
SS							loop				
AA						292	292	292	292		292
SS						loop	loop	loop	loop		loop
AA				299							
SS				H8							
AA								381	381		
SS								H11	H11		
AA								388			
SS								H11			
AA							401	401			
SS							H12	H12			
AA	HOH502/HOH 503/HOH504										
SS											

AA = Amino Acid      SS = Secondary Structure

Table 18  
Coordination Structure of TR- $\beta$  and Triac

Coordination Structure	R1	R2	R3	R5	R6	R2'	R3	R4	R5	R6	X
	-CH <sub>2</sub> CO <sub>2</sub> H	H	I	I	H	H	I	OH	H	H	O
AA							269				
SS							H3				
AA			272								
SS			H3								
AA			275								
SS			H3								
AA			276								
SS			H3								
AA	279	279									
SS	H3	H3									
AA				310					310	310	
SS				H5-H6					H5-H6	H5-H6	
AA	313				313						
SS	H5-H6				H5-H6						
AA	316										
SS	H5-H6										
AA	317				317		317				
SS	H5-H6				H5-H6		H5-H6				
AA	320										
SS	H5-H6										
AA	329										
SS	S3										
AA	330	330	330	330	330						
SS	S3	S3	S3	S3	S3						
AA	331										
SS	loop										
AA							344				
SS							loop				
AA							346	346			
SS							loop	loop			
AA				353							
SS				H8							
AA								435	435		
SS								H11	H11		
AA							442	442			
SS							H11	H11			
AA								455			
SS								H12			

AA = Amino Acid

SS = Secondary Structure

Table 19  
Coordination Structure of TR- $\beta$  and GC1

Coordination Structure	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>5</sub>	R <sub>6</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>4</sub>	R <sub>5</sub>	R <sub>6</sub>	X
	-O-CH <sub>2</sub> CO <sub>2</sub> H	H	CH <sub>3</sub>	CH <sub>3</sub>	H	H	CH(CH <sub>3</sub> )	OH	H	H	CH <sub>2</sub>
AA							269				
SS							H3				
AA			272								
SS			H3								
AA			273				273				
SS			H3				H3				
AA			275								
SS			H3								
AA			276					276	276	276	
SS			H3					H3	H3	H3	
AA	279	279									
SS	H3	H3									
AA	282										
SS	H3										
AA				310					310	310	
SS				H5-H6					H5-H6	H5-H6	
AA	313				313						
SS	H5-H6				H5-H6						
AA							314				
SS							H5-H6				
AA	316										
SS	H5-H6										
AA							317				
SS							H5-H6				
AA	320										
SS	H5-H6										
AA	329										
SS	S3										
AA	330			330							
SS	S3			S3							
AA	331										
SS	loop										
AA							344				
SS							loop				
AA							346	346			
SS							loop	loop			
AA				353							
SS				H8							
AA								435	435		
								H11	H11		
								455			
SS								H12			

AA = Amino Acid

SS = Secondary Structure

# APPENDIX 3

## TR\_DMT.PDB

REMARK TR\_dmt full length numbering

REMARK

REMARK Rfactor 0.205 Rfree 0.227

REMARK Resolution 15. 2.2 all reflections

REMARK

REMARK Three cacodylate-modified cysteines (CYA)

REMARK Cya334, Cya380, Cya392

REMARK cacodylate modeled as single arsenic atom

REMARK

REMARK side chain of certain residues modeled as ALA due to poor density;

REMARK however, residue name reflects true residue for clarity

REMARK

REMARK clone obtained from Murray et. al.

REMARK deposited sequence confirmed,

REMARK differing from that reported by Thompson et. al.

REMARK in the following codons:

REMARK 281 Thr - Ala

REMARK 285 Lys - Glu

REMARK identical to that reported by Mitsuhashi et. al.

REMARK gb:RNTRAVI X07409

JRNL AUTH M.B. MURRAY, N.D.ZILZ, N.L.MCCREARY,M.J.MACDONALD

JRNL AUTH 2 H.C.TOWLE

JRNL TITL ISOLATION AND CHARACTERIZATION OF RAT CDNA CLONES  
FOR TWO

JRNL TITL 2 DISTINCT THYROID HORMONE RECPTORS

JRNL REF JBC V. 263 25 1988

JRNL AUTH C.C.THOMPSON, C.WEINBERGER, R.LEBO, R.M.EVANS

JRNL TITL IDENTIFICATION OF A NOVEL THYROID HORMONE RECEPTOR  
EXPRESSED

JRNL TITL 2 IN THE MAMMALIAN CENTRAL NERVOUS SYSTEM

JRNL REF SCIENCE V. 237 1987

JRNL AUTH T.MITSUHASHI,G.TENNYSON,V.NIKODEM

JRNL TITL NUCLEOTIDE SEQUENCE OF NOVEL CDNAS GENERATED BY  
ALTERNATIVE

JRNL TITL 2 SPLICING OF A RAT THYROID HORMONE RECEPTOR GENE  
TRANSCRIPT

JRNL REF NUC. ACIDS. RES. V. 16 12 1988

ATOM 1 N ARG 157 68.504 8.445 5.651 1.00 68.93

ATOM 2 CA ARG 157 67.886 9.543 6.398 1.00 56.98

ATOM 3 CB ARG 157 68.769 10.789 6.324 1.00 59.25

ATOM 4 CG ARG 157 70.147 10.632 6.932 1.00 58.90



ATOM	5	CD	ARG	157	70.068	10.422	8.425	1.00	59.37
ATOM	6	NE	ARG	157	71.392	10.446	9.036	1.00	63.94
ATOM	7	CZ	ARG	157	71.613	10.329	10.341	1.00	64.39
ATOM	8	NH1	ARG	157	70.596	10.182	11.179	1.00	62.14
ATOM	9	NH2	ARG	157	72.855	10.365	10.808	1.00	65.56
ATOM	10	C -	ARG	157	66.500	9.881	5.854	1.00	48.97
ATOM	11	O	ARG	157	66.351	10.203	4.674	1.00	48.61
ATOM	12	N	PRO	158	65.469	9.818	6.712	1.00	41.90
ATOM	13	CD	PRO	158	65.550	9.366	8.112	1.00	41.06
ATOM	14	CA	PRO	158	64.083	10.114	6.333	1.00	39.34
ATOM	15	CB	PRO	158	63.286	9.704	7.576	1.00	37.89
ATOM	16	CG	PRO	158	64.260	9.883	8.693	1.00	42.40
ATOM	17	C	PRO	158	63.814	11.573	5.930	1.00	37.10
ATOM	18	O	PRO	158	64.189	12.517	6.636	1.00	33.31
ATOM	19	N	GLU	159	63.171	11.733	4.778	1.00	30.56
ATOM	20	CA	GLU	159	62.821	13.038	4.231	1.00	24.26
ATOM	21	CB	GLU	159	62.553	12.904	2.727	1.00	19.19
ATOM	22	CG	GLU	159	63.788	12.677	1.874	1.00	20.60
ATOM	23	CD	GLU	159	64.407	13.971	1.390	1.00	26.54
ATOM	24	OE1	GLU	159	63.649	14.929	1.115	1.00	30.85
ATOM	25	OE2	GLU	159	65.649	14.027	1.268	1.00	28.35
ATOM	26	C	GLU	159	61.549	13.520	4.909	1.00	23.26
ATOM	27	O	GLU	159	60.906	12.765	5.643	1.00	26.86
ATOM	28	N	PRO	160	61.200	14.806	4.729	1.00	22.72
ATOM	29	CD	PRO	160	61.981	15.916	4.153	1.00	17.87
ATOM	30	CA	PRO	160	59.969	15.292	5.359	1.00	19.90
ATOM	31	CB	PRO	160	60.004	16.799	5.070	1.00	14.42
ATOM	32	CG	PRO	160	61.465	17.109	4.919	1.00	12.87
ATOM	33	C	PRO	160	58.747	14.623	4.701	1.00	23.68
ATOM	34	O	PRO	160	58.730	14.383	3.491	1.00	24.72
ATOM	35	N	THR	161	57.749	14.281	5.506	1.00	22.19
ATOM	36	CA	THR	161	56.542	13.660	4.985	1.00	19.50
ATOM	37	CB	THR	161	55.691	13.031	6.125	1.00	21.50
ATOM	38	OG1	THR	161	55.163	14.062	6.972	1.00	20.33
ATOM	39	CG2	THR	161	56.537	12.078	6.959	1.00	19.48
ATOM	40	C	THR	161	55.744	14.765	4.298	1.00	22.86
ATOM	41	O	THR	161	56.040	15.949	4.481	1.00	27.68
ATOM	42	N	PRO	162	54.720	14.403	3.504	1.00	20.36
ATOM	43	CD	PRO	162	54.280	13.050	3.113	1.00	16.55
ATOM	44	CA	PRO	162	53.924	15.435	2.830	1.00	21.97
ATOM	45	CB	PRO	162	52.780	14.633	2.210	1.00	18.17
ATOM	46	CG	PRO	162	53.422	13.316	1.905	1.00	18.01
ATOM	47	C	PRO	162	53.399	16.467	3.826	1.00	22.56
ATOM	48	O	PRO	162	53.461	17.675	3.567	1.00	21.73
ATOM	49	N	GLU	163	52.912	15.976	4.967	1.00	25.28
ATOM	50	CA	GLU	163	52.357	16.816	6.030	1.00	26.64
ATOM	51	CB	GLU	163	51.743	15.9			



ATOM	52	CG	GLU	163	50.514	15.131	6.748	1.00	44.99
ATOM	53	CD	GLU	163	50.836	13.950	5.831	1.00	48.88
ATOM	54	OE1	GLU	163	50.016	13.660	4.929	1.00	52.48
ATOM	55	OE2	GLU	163	51.895	13.309	6.015	1.00	44.23
ATOM	56	C	GLU	163	53.414	17.731	6.634	1.00	27.65
ATOM	57	O -	GLU	163	53.114	18.862	7.034	1.00	29.30
ATOM	58	N	GLU	164	54.646	17.235	6.712	1.00	21.89
ATOM	59	CA	GLU	164	55.741	18.015	7.265	1.00	18.29
ATOM	60	CB	GLU	164	56.901	17.109	7.657	1.00	14.78
ATOM	61	CG	GLU	164	56.552	16.196	8.825	1.00	21.11
ATOM	62	CD	GLU	164	57.669	15.249	9.198	1.00	20.35
ATOM	63	OE1	GLU	164	58.605	15.071	8.392	1.00	28.55
ATOM	64	OE2	GLU	164	57.610	14.677	10.302	1.00	28.25
ATOM	65	C	GLU	164	56.200	19.097	6.306	1.00	24.62
ATOM	66	O	GLU	164	56.574	20.183	6.741	1.00	32.05
ATOM	67	N	TRP	165	56.174	18.817	5.003	1.00	28.22
ATOM	68	CA	TRP	165	56.576	19.825	4.021	1.00	22.99
ATOM	69	CB	TRP	165	56.575	19.262	2.605	1.00	17.37
ATOM	70	CG	TRP	165	57.876	18.633	2.210	1.00	10.74
ATOM	71	CD2	TRP	165	59.153	19.283	2.109	1.00	11.74
ATOM	72	CE2	TRP	165	60.075	18.319	1.648	1.00	9.97
ATOM	73	CE3	TRP	165	59.606	20.583	2.365	1.00	13.88
ATOM	74	CD1	TRP	165	58.074	17.343	1.832	1.00	9.17
ATOM	75	NE1	TRP	165	59.390	17.145	1.486	1.00	16.55
ATOM	76	CZ2	TRP	165	61.427	18.613	1.436	1.00	13.37
ATOM	77	CZ3	TRP	165	60.954	20.874	2.156	1.00	16.15
ATOM	78	CH2	TRP	165	61.846	19.892	1.696	1.00	17.42
ATOM	79	C	TRP	165	55.634	21.015	4.115	1.00	21.44
ATOM	80	O	TRP	165	56.041	22.149	3.865	1.00	22.12
ATOM	81	N	ASP	166	54.373	20.747	4.456	1.00	21.29
ATOM	82	CA	ASP	166	53.369	21.796	4.621	1.00	25.77
ATOM	83	CB	ASP	166	51.972	21.196	4.808	1.00	26.02
ATOM	84	CG	ASP	166	51.428	20.559	3.539	1.00	33.01
ATOM	85	OD1	ASP	166	51.874	20.932	2.434	1.00	29.48
ATOM	86	OD2	ASP	166	50.537	19.692	3.649	1.00	34.47
ATOM	87	C	ASP	166	53.732	22.637	5.842	1.00	27.91
ATOM	88	O	ASP	166	53.744	23.865	5.767	1.00	31.28
ATOM	89	N	LEU	167	54.046	21.966	6.951	1.00	25.57
ATOM	90	CA	LEU	167	54.439	22.640	8.187	1.00	28.28
ATOM	91	CB	LEU	167	54.854	21.624	9.256	1.00	32.80
ATOM	92	CG	LEU	167	53.945	21.347	10.455	1.00	41.75
ATOM	93	CD1	LEU	167	54.765	20.640	11.532	1.00	39.15
ATOM	94	CD2	LEU	167	53.374	22.647	11.008	1.00	39.20
ATOM	95	C	LEU	167	55.636	23.532	7.902	1.00	22.19
ATOM	96	O	LEU	167	55.671	24.700	8.302	1.00	29.51
ATOM	97	N	ILE	168	56.610	22.957	7.206	1.00	15.01
ATOM									

ATOM	99	CB	ILE	168	58.756	22.668	6.040	1.00	11.37
ATOM	100	CG2	ILE	168	59.890	23.413	5.367	1.00	16.36
ATOM	101	CG1	ILE	168	59.289	21.580	6.975	1.00	21.63
ATOM	102	CD1	ILE	168	60.095	20.501	6.287	1.00	21.03
ATOM	103	C	ILE	168	57.579	24.897	6.022	1.00	22.54
ATOM	104	O-	ILE	168	58.155	25.948	6.300	1.00	24.88
ATOM	105	N	HIS	169	56.682	24.800	5.045	1.00	25.70
ATOM	106	CA	HIS	169	56.337	25.934	4.190	1.00	21.28
ATOM	107	CB	HIS	169	55.411	25.493	3.057	1.00	22.29
ATOM	108	CG	HIS	169	56.047	24.543	2.091	1.00	23.11
ATOM	109	CD2	HIS	169	57.348	24.265	1.839	1.00	16.86
ATOM	110	ND1	HIS	169	55.312	23.721	1.263	1.00	25.30
ATOM	111	CE1	HIS	169	56.130	22.974	0.546	1.00	15.89
ATOM	112	NE2	HIS	169	57.371	23.283	0.878	1.00	25.38
ATOM	113	C	HIS	169	55.664	27.048	4.976	1.00	18.32
ATOM	114	O	HIS	169	56.033	28.215	4.842	1.00	21.53
ATOM	115	N	VAL	170	54.679	26.685	5.795	1.00	17.13
ATOM	116	CA	VAL	170	53.957	27.661	6.607	1.00	21.29
ATOM	117	CB	VAL	170	52.808	26.991	7.399	1.00	24.33
ATOM	118	CG1	VAL	170	52.164	27.985	8.354	1.00	23.78
ATOM	119	CG2	VAL	170	51.760	26.439	6.435	1.00	18.87
ATOM	120	C	VAL	170	54.910	28.382	7.567	1.00	24.69
ATOM	121	O	VAL	170	54.912	29.616	7.637	1.00	28.77
ATOM	122	N	ALA	171	55.759	27.609	8.245	1.00	20.35
ATOM	123	CA	ALA	171	56.722	28.148	9.202	1.00	19.61
ATOM	124	CB	ALA	171	57.393	27.013	9.977	1.00	17.52
ATOM	125	C	ALA	171	57.775	29.026	8.531	1.00	20.91
ATOM	126	O	ALA	171	58.102	30.105	9.041	1.00	21.98
ATOM	127	N	THR	172	58.308	28.571	7.398	1.00	18.94
ATOM	128	CA	THR	172	59.313	29.342	6.668	1.00	19.55
ATOM	129	CB	THR	172	59.820	28.594	5.413	1.00	20.49
ATOM	130	OG1	THR	172	60.394	27.336	5.795	1.00	20.66
ATOM	131	CG2	THR	172	60.894	29.418	4.702	1.00	20.44
ATOM	132	C	THR	172	58.730	30.697	6.254	1.00	23.26
ATOM	133	O	THR	172	59.403	31.724	6.334	1.00	24.32
ATOM	134	N	GLU	173	57.468	30.694	5.836	1.00	27.42
ATOM	135	CA	GLU	173	56.797	31.922	5.434	1.00	27.68
ATOM	136	CB	GLU	173	55.477	31.605	4.728	1.00	24.51
ATOM	137	CG	GLU	173	54.652	32.836	4.338	1.00	39.69
ATOM	138	CD	GLU	173	55.396	33.814	3.426	1.00	47.72
ATOM	139	OE1	GLU	173	55.019	35.009	3.417	1.00	48.26
ATOM	140	OE2	GLU	173	56.344	33.398	2.717	1.00	49.61
ATOM	141	C	GLU	173	56.557	32.834	6.641	1.00	25.68
ATOM	142	O	GLU	173	56.773	34.046	6.559	1.00	23.39
ATOM	143	N	ALA	174	56.119	32.245	7.755	1.00	25.19
ATOM	144	CA	ALA	174	55.863	32.989	8.993	1.00	22.25

ATOM	146	C	ALA	174	57.125	33.747	9.391	1.00	23.22
ATOM	147	O	ALA	174	57.076	34.918	9.768	1.00	24.52
ATOM	148	N	HIS	175	58.261	33.073	9.275	1.00	20.97
ATOM	149	CA	HIS	175	59.544	33.665	9.606	1.00	19.55
ATOM	150	CB	HIS	175	60.625	32.577	9.649	1.00	16.19
ATOM	151	CG	HIS	175	62.016	33.104	9.835	1.00	18.89
ATOM	152	CD2	HIS	175	63.148	32.901	9.119	1.00	16.05
ATOM	153	ND1	HIS	175	62.359	33.962	10.859	1.00	13.83
ATOM	154	CE1	HIS	175	63.642	34.265	10.765	1.00	15.87
ATOM	155	NE2	HIS	175	64.143	33.635	9.718	1.00	19.19
ATOM	156	C	HIS	175	59.934	34.757	8.617	1.00	21.28
ATOM	157	O	HIS	175	60.274	35.869	9.014	1.00	25.12
ATOM	158	N	ARG	176	59.891	34.436	7.329	1.00	26.73
ATOM	159	CA	ARG	176	60.266	35.387	6.292	1.00	27.13
ATOM	160	CB	ARG	176	60.156	34.748	4.914	1.00	36.00
ATOM	161	CG	ARG	176	61.286	33.795	4.602	1.00	43.20
ATOM	162	CD	ARG	176	61.197	33.334	3.170	1.00	50.07
ATOM	163	NE	ARG	176	62.316	32.477	2.813	1.00	58.20
ATOM	164	CZ	ARG	176	62.266	31.548	1.867	1.00	67.22
ATOM	165	NH1	ARG	176	61.143	31.358	1.182	1.00	67.62
ATOM	166	NH2	ARG	176	63.336	30.806	1.612	1.00	70.56
ATOM	167	C	ARG	176	59.487	36.688	6.325	1.00	23.97
ATOM	168	O	ARG	176	60.073	37.760	6.209	1.00	24.52
ATOM	169	N	SER	177	58.177	36.598	6.515	1.00	23.60
ATOM	170	CA	SER	177	57.341	37.789	6.565	1.00	26.36
ATOM	171	CB	SER	177	55.865	37.407	6.439	1.00	21.93
ATOM	172	OG	SER	177	55.495	36.459	7.423	1.00	25.97
ATOM	173	C	SER	177	57.557	38.623	7.829	1.00	28.76
ATOM	174	O	SER	177	57.084	39.761	7.907	1.00	33.09
ATOM	175	N	THR	178	58.257	38.062	8.815	1.00	25.52
ATOM	176	CA	THR	178	58.508	38.772	10.064	1.00	18.93
ATOM	177	CB	THR	178	57.828	38.064	11.258	1.00	21.81
ATOM	178	OG1	THR	178	58.348	36.736	11.394	1.00	24.18
ATOM	179	CG2	THR	178	56.330	37.971	11.032	1.00	13.81
ATOM	180	C	THR	178	59.993	38.967	10.358	1.00	20.69
ATOM	181	O	THR	178	60.373	39.407	11.448	1.00	20.56
ATOM	182	N	ASN	179	60.837	38.645	9.385	1.00	23.68
ATOM	183	CA	ASN	179	62.275	38.802	9.555	1.00	28.22
ATOM	184	CB	ASN	179	63.022	37.627	8.927	1.00	27.45
ATOM	185	CG	ASN	179	64.460	37.529	9.402	1.00	33.98
ATOM	186	OD1	ASN	179	65.342	37.131	8.644	1.00	42.72
ATOM	187	ND2	ASN	179	64.702	37.865	10.667	1.00	31.14
ATOM	188	C	ASN	179	62.689	40.115	8.902	1.00	34.47
ATOM	189	O	ASN	179	62.832	40.200	7.678	1.00	36.54
ATOM	190	N	ALA	180	62.874	41.135	9.735	1.00	37.39
ATOM	191	CA	ALA	180	63.235	42.479	9.292	1.00	33.71

ATOM	193	C	ALA	180	64.375	42.545	8.284	1.00	37.87
ATOM	194	O	ALA	180	65.458	42.018	8.525	1.00	35.26
ATOM	195	N	GLN	181	64.095	43.187	7.150	1.00	40.55
ATOM	196	CA	GLN	181	65.049	43.391	6.057	1.00	42.95
ATOM	197	CB	GLN	181	66.344	44.043	6.570	1.00	45.47
ATOM	198	CG	GLN	181	66.144	45.326	7.383	1.00	52.70
ATOM	199	CD	GLN	181	65.351	46.399	6.650	1.00	55.03
ATOM	200	OE1	GLN	181	65.270	46.412	5.421	1.00	59.56
ATOM	201	NE2	GLN	181	64.757	47.308	7.411	1.00	54.39
ATOM	202	C	GLN	181	65.391	42.176	5.197	1.00	44.27
ATOM	203	O	GLN	181	66.181	42.291	4.251	1.00	46.47
ATOM	204	N	GLY	182	64.797	41.025	5.508	1.00	42.17
ATOM	205	CA	GLY	182	65.054	39.815	4.742	1.00	42.63
ATOM	206	C	GLY	182	66.522	39.584	4.427	1.00	47.40
ATOM	207	O	GLY	182	67.382	39.691	5.306	1.00	49.38
ATOM	208	N	SER	183	66.816	39.297	3.163	1.00	49.46
ATOM	209	CA	SER	183	68.189	39.061	2.733	1.00	54.13
ATOM	210	CB	SER	183	68.208	38.225	1.449	1.00	55.08
ATOM	211	OG	SER	183	67.197	38.647	0.546	1.00	63.54
ATOM	212	C	SER	183	68.949	40.369	2.532	1.00	54.84
ATOM	213	O	SER	183	70.175	40.373	2.407	1.00	56.90
ATOM	214	N	HIS	184	68.223	41.482	2.535	1.00	55.77
ATOM	215	CA	HIS	184	68.854	42.775	2.342	1.00	57.78
ATOM	216	C	HIS	184	69.605	43.296	3.556	1.00	59.09
ATOM	217	O	HIS	184	70.312	44.301	3.454	1.00	60.34
ATOM	218	N	TRP	185	69.502	42.597	4.686	1.00	55.60
ATOM	219	CA	TRP	185	70.159	43.020	5.923	1.00	53.73
ATOM	220	CB	TRP	185	69.973	41.973	7.030	1.00	50.40
ATOM	221	CG	TRP	185	70.746	40.694	6.837	1.00	48.09
ATOM	222	CD2	TRP	185	72.091	40.419	7.269	1.00	47.38
ATOM	223	CE2	TRP	185	72.390	39.094	6.888	1.00	40.29
ATOM	224	CE3	TRP	185	73.071	41.169	7.937	1.00	45.43
ATOM	225	CD1	TRP	185	70.301	39.554	6.234	1.00	49.87
ATOM	226	NE1	TRP	185	71.280	38.589	6.262	1.00	48.02
ATOM	227	CZ2	TRP	185	73.628	38.496	7.154	1.00	38.65
ATOM	228	CZ3	TRP	185	74.304	40.573	8.201	1.00	43.26
ATOM	229	CH2	TRP	185	74.570	39.250	7.807	1.00	40.00
ATOM	230	C	TRP	185	71.638	43.386	5.800	1.00	55.99
ATOM	231	O	TRP	185	72.089	44.359	6.401	1.00	52.84
ATOM	232	N	LYS	186	72.389	42.614	5.021	1.00	59.15
ATOM	233	CA	LYS	186	73.818	42.863	4.843	1.00	64.01
ATOM	234	CB	LYS	186	74.466	41.688	4.091	1.00	64.67
ATOM	235	CG	LYS	186	75.943	41.868	3.729	1.00	65.58
ATOM	236	CD	LYS	186	76.817	42.181	4.946	1.00	62.03
ATOM	237	CE	LYS	186	78.238	42.512	4.515	1.00	61.52
ATOM	238	NZ	LYS	186	78.988	43.243	5.5		



ATOM	240	O	LYS	186	75.164	44.816	4.432	1.00	68.66
ATOM	241	N	GLN	187	73.221	44.678	3.316	1.00	68.99
ATOM	242	CA	GLN	187	73.431	45.939	2.612	1.00	69.65
ATOM	243	CB	GLN	187	72.880	45.867	1.180	1.00	73.76
ATOM	244	CG	GLN	187	73.632	44.935	0.237	1.00	78.61
ATOM	245	CD	GLN	187	73.368	43.471	0.525	1.00	84.96
ATOM	246	OE1	GLN	187	74.203	42.782	1.109	1.00	87.73
ATOM	247	NE2	GLN	187	72.197	42.989	0.122	1.00	84.98
ATOM	248	C	GLN	187	72.817	47.141	3.323	1.00	69.16
ATOM	249	O	GLN	187	73.379	48.235	3.299	1.00	71.39
ATOM	250	N	ARG	188	71.666	46.936	3.953	1.00	65.82
ATOM	251	CA	ARG	188	70.961	48.014	4.639	1.00	65.00
ATOM	252	CB	ARG	188	69.458	47.739	4.591	1.00	66.20
ATOM	253	CG	ARG	188	68.957	47.483	3.181	1.00	70.30
ATOM	254	CD	ARG	188	67.463	47.212	3.132	1.00	78.59
ATOM	255	NE	ARG	188	67.003	47.008	1.760	1.00	87.71
ATOM	256	CZ	ARG	188	67.011	47.946	0.814	1.00	94.10
ATOM	257	NH1	ARG	188	67.453	49.171	1.081	1.00	97.26
ATOM	258	NH2	ARG	188	66.589	47.657	-0.409	1.00	94.07
ATOM	259	C	ARG	188	71.409	48.286	6.077	1.00	65.39
ATOM	260	O	ARG	188	70.900	49.201	6.727	1.00	65.20
ATOM	261	N	ARG	189	72.372	47.506	6.561	1.00	64.28
ATOM	262	CA	ARG	189	72.882	47.654	7.922	1.00	60.75
ATOM	263	CB	ARG	189	73.691	46.409	8.321	1.00	56.87
ATOM	264	CG	ARG	189	75.050	46.308	7.630	1.00	59.52
ATOM	265	CD	ARG	189	75.580	44.891	7.589	1.00	55.86
ATOM	266	NE	ARG	189	75.874	44.348	8.907	1.00	55.48
ATOM	267	CZ	ARG	189	77.055	43.849	9.257	1.00	61.38
ATOM	268	NH1	ARG	189	78.057	43.832	8.388	1.00	62.54
ATOM	269	NH2	ARG	189	77.225	43.328	10.465	1.00	62.20
ATOM	270	C	ARG	189	73.747	48.907	8.082	1.00	60.91
ATOM	271	O	ARG	189	74.548	49.245	7.207	1.00	60.67
ATOM	272	N	LYS	190	73.575	49.591	9.207	1.00	59.06
ATOM	273	CA	LYS	190	74.340	50.790	9.521	1.00	55.00
ATOM	274	CB	LYS	190	73.423	52.008	9.582	1.00	55.45
ATOM	275	C	LYS	190	74.991	50.542	10.875	1.00	51.52
ATOM	276	O	LYS	190	74.320	50.144	11.830	1.00	51.68
ATOM	277	N	PHE	191	76.304	50.721	10.944	1.00	50.49
ATOM	278	CA	PHE	191	77.037	50.508	12.186	1.00	50.17
ATOM	279	CB	PHE	191	78.546	50.571	11.943	1.00	48.38
ATOM	280	CG	PHE	191	79.090	49.423	11.142	1.00	49.66
ATOM	281	CD1	PHE	191	78.873	49.348	9.768	1.00	51.03
ATOM	282	CD2	PHE	191	79.845	48.429	11.759	1.00	46.28
ATOM	283	CE1	PHE	191	79.403	48.298	9.018	1.00	51.35
ATOM	284	CE2	PHE	191	80.379	47.377	11.021	1.00	47.26
ATOM	285	CZ	PHE	191	80.158	47.311	9.646		

ATOM	287	O	PHE	191	76.507	52.720	12.952	1.00	50.38
ATOM	288	N	LEU	192	76.488	51.068	14.479	1.00	47.31
ATOM	289	CA	LEU	192	76.169	51.958	15.584	1.00	42.72
ATOM	290	CB	LEU	192	75.845	51.151	16.844	1.00	36.66
ATOM	291	CG	LEU	192	75.397	51.949	18.068	1.00	31.01
ATOM	292	CD1	LEU	192	74.048	52.590	17.786	1.00	28.37
ATOM	293	CD2	LEU	192	75.318	51.043	19.289	1.00	29.60
ATOM	294	C	LEU	192	77.447	52.760	15.800	1.00	42.28
ATOM	295	O	LEU	192	78.528	52.179	15.932	1.00	39.71
ATOM	296	N	PRO	193	77.350	54.104	15.781	1.00	45.15
ATOM	297	CD	PRO	193	76.095	54.865	15.617	1.00	43.82
ATOM	298	CA	PRO	193	78.493	55.006	15.973	1.00	43.14
ATOM	299	CB	PRO	193	77.820	56.306	16.400	1.00	44.37
ATOM	300	CG	PRO	193	76.571	56.308	15.565	1.00	41.66
ATOM	301	C	PRO	193	79.476	54.498	17.028	1.00	43.34
ATOM	302	O	PRO	193	79.103	54.296	18.182	1.00	45.18
ATOM	303	N	ASP	194	80.732	54.317	16.628	1.00	44.22
ATOM	304	CA	ASP	194	81.781	53.804	17.512	1.00	47.20
ATOM	305	CB	ASP	194	83.108	53.732	16.761	1.00	41.89
ATOM	306	C	ASP	194	81.962	54.511	18.866	1.00	51.99
ATOM	307	O	ASP	194	82.636	53.986	19.752	1.00	54.04
ATOM	308	N	ASP	195	81.381	55.698	19.025	1.00	55.21
ATOM	309	CA	ASP	195	81.489	56.428	20.288	1.00	57.50
ATOM	310	CB	ASP	195	81.423	57.948	20.061	1.00	60.04
ATOM	311	CG	ASP	195	80.123	58.398	19.406	1.00	68.39
ATOM	312	OD1	ASP	195	79.211	58.847	20.136	1.00	69.46
ATOM	313	OD2	ASP	195	80.020	58.322	18.162	1.00	72.91
ATOM	314	C	ASP	195	80.410	55.976	21.280	1.00	58.05
ATOM	315	O	ASP	195	80.540	56.180	22.491	1.00	58.97
ATOM	316	N	ILE	196	79.349	55.363	20.759	1.00	56.06
ATOM	317	CA	ILE	196	78.247	54.863	21.580	1.00	50.48
ATOM	318	CB	ILE	196	76.930	54.762	20.766	1.00	45.82
ATOM	319	CG2	ILE	196	75.818	54.166	21.621	1.00	44.04
ATOM	320	CG1	ILE	196	76.517	56.147	20.261	1.00	44.27
ATOM	321	CD1	ILE	196	75.179	56.171	19.541	1.00	45.25
ATOM	322	C	ILE	196	78.603	53.484	22.135	1.00	47.66
ATOM	323	O	ILE	196	79.138	52.636	21.419	1.00	43.96
ATOM	324	N	GLY	197	78.309	53.269	23.414	1.00	46.29
ATOM	325	CA	GLY	197	78.608	51.995	24.045	1.00	48.03
ATOM	326	C	GLY	197	79.978	51.963	24.692	1.00	50.42
ATOM	327	O	GLY	197	80.463	50.902	25.070	1.00	46.66
ATOM	328	N	GLN	198	80.583	53.137	24.854	1.00	56.94
ATOM	329	CA	GLN	198	81.910	53.259	25.454	1.00	59.51
ATOM	330	CB	GLN	198	82.751	54.257	24.649	1.00	62.53
ATOM	331	CG	GLN	198	83.232	53.718	23.316	1.00	69.39
ATOM	332	CD	GLN	198	84				



ATOM	334	NE2	GLN	198	85.205	52.632	24.192	1.00	78.09
ATOM	335	C	GLN	198	81.915	53.678	26.922	1.00	57.56
ATOM	336	O	GLN	198	82.946	53.584	27.588	1.00	57.71
ATOM	337	N	SER	199	80.770	54.128	27.425	1.00	54.11
ATOM	338	CA	SER	199	80.676	54.600	28.800	1.00	46.28
ATOM	339	CB	SER	199	80.243	56.067	28.777	1.00	50.28
ATOM	340	OG	SER	199	80.935	56.776	27.757	1.00	50.95
ATOM	341	C	SER	199	79.776	53.805	29.757	1.00	40.19
ATOM	342	O	SER	199	78.680	54.252	30.102	1.00	39.26
ATOM	343	N	PRO	200	80.236	52.629	30.214	1.00	35.63
ATOM	344	CD	PRO	200	81.530	52.011	29.904	1.00	34.88
ATOM	345	CA	PRO	200	79.464	51.789	31.139	1.00	37.54
ATOM	346	CB	PRO	200	80.223	50.457	31.124	1.00	29.86
ATOM	347	CG	PRO	200	81.207	50.570	29.995	1.00	34.29
ATOM	348	C	PRO	200	79.521	52.416	32.532	1.00	44.63
ATOM	349	O	PRO	200	80.443	52.137	33.300	1.00	47.80
ATOM	350	N	ILE	201	78.532	53.241	32.867	1.00	49.57
ATOM	351	CA	ILE	201	78.525	53.924	34.158	1.00	49.15
ATOM	352	CB	ILE	201	78.213	55.426	33.990	1.00	49.19
ATOM	353	CG2	ILE	201	78.429	56.150	35.306	1.00	53.37
ATOM	354	CG1	ILE	201	79.137	56.037	32.934	1.00	52.55
ATOM	355	CD1	ILE	201	78.811	57.471	32.586	1.00	55.26
ATOM	356	C	ILE	201	77.625	53.352	35.254	1.00	49.88
ATOM	357	O	ILE	201	78.044	53.250	36.408	1.00	50.20
ATOM	358	N	VAL	202	76.384	53.014	34.920	1.00	47.85
ATOM	359	CA	VAL	202	75.468	52.474	35.927	1.00	45.76
ATOM	360	CB	VAL	202	74.015	52.415	35.400	1.00	39.98
ATOM	361	CG1	VAL	202	73.072	51.896	36.482	1.00	35.94
ATOM	362	CG2	VAL	202	73.574	53.799	34.944	1.00	29.43
ATOM	363	C	VAL	202	75.954	51.093	36.373	1.00	50.57
ATOM	364	O	VAL	202	76.296	50.249	35.545	1.00	49.50
ATOM	365	N	SER	203	76.009	50.876	37.683	1.00	54.82
ATOM	366	CA	SER	203	76.490	49.609	38.223	1.00	59.26
ATOM	367	CB	SER	203	77.067	49.809	39.628	1.00	64.88
ATOM	368	OG	SER	203	76.127	50.428	40.492	1.00	75.47
ATOM	369	C	SER	203	75.457	48.491	38.244	1.00	55.78
ATOM	370	O	SER	203	74.285	48.712	38.544	1.00	57.50
ATOM	371	N	MET	204	75.923	47.283	37.958	1.00	52.29
ATOM	372	CA	MET	204	75.076	46.103	37.948	1.00	50.42
ATOM	373	CB	MET	204	75.032	45.487	36.548	1.00	47.74
ATOM	374	CG	MET	204	74.243	46.297	35.541	1.00	43.40
ATOM	375	SD	MET	204	72.491	46.348	35.953	1.00	40.93
ATOM	376	CE	MET	204	71.947	44.785	35.241	1.00	39.19
ATOM	377	C	MET	204	75.670	45.107	38.925	1.00	49.42
ATOM	378	O	MET	204	76.892	45.020	39.062	1.00	52.25
ATOM	379	N	PRO	205	74.816	44.329</			

ATOM	381	CA	PRO	205	75.250	43.326	40.580	1.00	47.34
ATOM	382	CB	PRO	205	73.982	42.513	40.810	1.00	49.44
ATOM	383	CG	PRO	205	72.907	43.562	40.725	1.00	50.62
ATOM	384	C	PRO	205	76.431	42.442	40.168	1.00	47.12
ATOM	385	O	PRO	205	77.299	42.160	40.990	1.00	51.21
ATOM	386	N	ASP	206	76.487	42.023	38.909	1.00	48.81
ATOM	387	CA	ASP	206	77.583	41.160	38.465	1.00	49.88
ATOM	388	CB	ASP	206	77.128	40.223	37.330	1.00	54.06
ATOM	389	CG	ASP	206	76.598	40.967	36.107	1.00	57.34
ATOM	390	OD1	ASP	206	77.056	42.095	35.811	1.00	52.21
ATOM	391	OD2	ASP	206	75.719	40.397	35.423	1.00	59.16
ATOM	392	C	ASP	206	78.902	41.843	38.093	1.00	48.70
ATOM	393	O	ASP	206	79.862	41.171	37.715	1.00	49.75
ATOM	394	N	GLY	207	78.946	43.168	38.161	1.00	47.54
ATOM	395	CA	GLY	207	80.174	43.869	37.820	1.00	49.23
ATOM	396	C	GLY	207	80.169	44.585	36.482	1.00	51.96
ATOM	397	O	GLY	207	80.783	45.645	36.348	1.00	56.32
ATOM	398	N	ASP	208	79.510	44.005	35.481	1.00	52.50
ATOM	399	CA	ASP	208	79.435	44.624	34.157	1.00	48.00
ATOM	400	CB	ASP	208	78.968	43.609	33.115	1.00	53.23
ATOM	401	CG	ASP	208	80.038	42.592	32.774	1.00	53.17
ATOM	402	OD1	ASP	208	81.130	43.006	32.335	1.00	57.42
ATOM	403	OD2	ASP	208	79.787	41.380	32.942	1.00	55.64
ATOM	404	C	ASP	208	78.497	45.823	34.187	1.00	46.68
ATOM	405	O	ASP	208	77.283	45.671	34.332	1.00	45.81
ATOM	406	N	LYS	209	79.075	47.014	34.077	1.00	45.95
ATOM	407	CA	LYS	209	78.313	48.257	34.115	1.00	45.87
ATOM	408	CB	LYS	209	79.235	49.418	34.478	1.00	46.90
ATOM	409	C	LYS	209	77.561	48.546	32.812	1.00	41.17
ATOM	410	O	LYS	209	77.951	48.074	31.745	1.00	39.51
ATOM	411	N	VAL	210	76.500	49.344	32.916	1.00	39.35
ATOM	412	CA	VAL	210	75.652	49.713	31.782	1.00	38.03
ATOM	413	CB	VAL	210	74.136	49.584	32.140	1.00	32.13
ATOM	414	CG1	VAL	210	73.269	49.926	30.937	1.00	27.92
ATOM	415	CG2	VAL	210	73.818	48.183	32.627	1.00	29.43
ATOM	416	C	VAL	210	75.895	51.134	31.263	1.00	38.68
ATOM	417	O	VAL	210	76.090	52.079	32.038	1.00	39.57
ATOM	418	N	ASP	211	75.848	51.272	29.942	1.00	39.19
ATOM	419	CA	ASP	211	76.019	52.544	29.254	1.00	38.39
ATOM	420	CB	ASP	211	76.794	52.327	27.946	1.00	40.36
ATOM	421	CG	ASP	211	77.051	53.620	27.177	1.00	36.85
ATOM	422	OD1	ASP	211	76.193	54.528	27.167	1.00	37.95
ATOM	423	OD2	ASP	211	78.121	53.716	26.553	1.00	33.87
ATOM	424	C	ASP	211	74.601	53.040	28.958	1.00	40.60
ATOM	425	O	ASP	211	73.919	52.517	28.073	1.00	40.36
ATOM	426	N	LEU	212	74.185	54.074	29.680	1.00	41.55
ATOM	427	CA	LEU	212	72.854	54.664	29.552	1.00	38.39

ATOM	428	CB	LEU	212	72.759	55.883	30.467	1.00	40.93
ATOM	429	CG	LEU	212	71.575	55.979	31.428	1.00	45.32
ATOM	430	CD1	LEU	212	71.271	54.626	32.047	1.00	43.83
ATOM	431	CD2	LEU	212	71.900	57.007	32.502	1.00	44.93
ATOM	432	C	LEU	212	72.448	55.050	28.133	1.00	37.61
ATOM	433	O <sup>-</sup>	LEU	212	71.318	54.805	27.719	1.00	33.71
ATOM	434	N	GLU	213	73.360	55.670	27.393	1.00	41.23
ATOM	435	CA	GLU	213	73.068	56.084	26.023	1.00	43.48
ATOM	436	CB	GLU	213	74.181	56.986	25.481	1.00	47.66
ATOM	437	CG	GLU	213	73.919	57.494	24.065	1.00	56.87
ATOM	438	CD	GLU	213	75.121	58.180	23.433	1.00	60.87
ATOM	439	OE1	GLU	213	76.258	57.996	23.924	1.00	60.37
ATOM	440	OE2	GLU	213	74.921	58.894	22.423	1.00	61.13
ATOM	441	C	GLU	213	72.889	54.880	25.102	1.00	39.29
ATOM	442	O	GLU	213	71.965	54.841	24.290	1.00	36.66
ATOM	443	N	ALA	214	73.785	53.906	25.233	1.00	36.33
ATOM	444	CA	ALA	214	73.739	52.693	24.422	1.00	34.89
ATOM	445	CB	ALA	214	74.946	51.817	24.711	1.00	30.70
ATOM	446	C	ALA	214	72.454	51.938	24.718	1.00	31.96
ATOM	447	O	ALA	214	71.739	51.523	23.804	1.00	33.93
ATOM	448	N	PHE	215	72.151	51.798	26.003	1.00	28.47
ATOM	449	CA	PHE	215	70.947	51.116	26.445	1.00	29.74
ATOM	450	CB	PHE	215	70.819	51.223	27.962	1.00	23.73
ATOM	451	CG	PHE	215	69.589	50.568	28.515	1.00	22.71
ATOM	452	CD1	PHE	215	69.603	49.220	28.858	1.00	22.53
ATOM	453	CD2	PHE	215	68.423	51.301	28.712	1.00	19.74
ATOM	454	CE1	PHE	215	68.477	48.606	29.391	1.00	20.75
ATOM	455	CE2	PHE	215	67.290	50.698	29.245	1.00	21.02
ATOM	456	CZ	PHE	215	67.318	49.346	29.586	1.00	19.50
ATOM	457	C	PHE	215	69.730	51.742	25.771	1.00	34.64
ATOM	458	O	PHE	215	68.872	51.034	25.239	1.00	39.86
ATOM	459	N	SER	216	69.677	53.071	25.771	1.00	34.78
ATOM	460	CA	SER	216	68.572	53.801	25.160	1.00	36.01
ATOM	461	CB	SER	216	68.762	55.302	25.366	1.00	37.36
ATOM	462	OG	SER	216	67.537	55.987	25.193	1.00	48.33
ATOM	463	C	SER	216	68.458	53.475	23.664	1.00	37.06
ATOM	464	O	SER	216	67.358	53.250	23.148	1.00	33.23
ATOM	465	N	GLU	217	69.601	53.410	22.986	1.00	36.25
ATOM	466	CA	GLU	217	69.645	53.091	21.562	1.00	36.99
ATOM	467	CB	GLU	217	71.092	53.104	21.064	1.00	37.10
ATOM	468	CG	GLU	217	71.682	54.491	20.912	1.00	44.30
ATOM	469	CD	GLU	217	71.016	55.284	19.802	1.00	51.30
ATOM	470	OE1	GLU	217	71.439	55.142	18.633	1.00	57.25
ATOM	471	OE2	GLU	217	70.070	56.046	20.096	1.00	52.50
ATOM	472	C	GLU	217	69.019	51.726	21.286	1.00	36.93
ATOM	473	O							

ATOM	475	CA	PHE	218	68.875	49.388	21.947	1.00	27.20
ATOM	476	CB	PHE	218	69.679	48.421	22.814	1.00	28.10
ATOM	477	CG	PHE	218	71.124	48.330	22.428	1.00	24.84
ATOM	478	CD1	PHE	218	72.117	48.286	23.398	1.00	21.78
ATOM	479	CD2	PHE	218	71.495	48.301	21.087	1.00	24.78
ATOM	480	CE1	PHE	218	73.458	48.215	23.040	1.00	24.08
ATOM	481	CE2	PHE	218	72.834	48.230	20.719	1.00	25.33
ATOM	482	CZ	PHE	218	73.818	48.187	21.697	1.00	25.04
ATOM	483	C	PHE	218	67.381	49.281	22.261	1.00	28.23
ATOM	484	O	PHE	218	66.639	48.605	21.543	1.00	33.52
ATOM	485	N	THR	219	66.927	49.961	23.310	1.00	27.24
ATOM	486	CA	THR	219	65.515	49.913	23.666	1.00	29.28
ATOM	487	CB	THR	219	65.238	50.533	25.052	1.00	30.97
ATOM	488	OG1	THR	219	65.724	51.880	25.090	1.00	35.50
ATOM	489	CG2	THR	219	65.901	49.712	26.149	1.00	30.78
ATOM	490	C	THR	219	64.660	50.612	22.615	1.00	33.29
ATOM	491	O	THR	219	63.473	50.317	22.474	1.00	36.85
ATOM	492	N	LYS	220	65.276	51.515	21.860	1.00	35.23
ATOM	493	CA	LYS	220	64.579	52.253	20.816	1.00	38.97
ATOM	494	CB	LYS	220	65.506	53.334	20.236	1.00	44.67
ATOM	495	CG	LYS	220	64.805	54.491	19.513	1.00	58.02
ATOM	496	CD	LYS	220	64.406	54.130	18.079	1.00	68.57
ATOM	497	CE	LYS	220	63.732	55.296	17.347	1.00	70.50
ATOM	498	NZ	LYS	220	62.395	55.668	17.905	1.00	66.08
ATOM	499	C	LYS	220	64.112	51.289	19.721	1.00	38.48
ATOM	500	O	LYS	220	63.021	51.446	19.173	1.00	37.18
ATOM	501	N	ILE	221	64.917	50.270	19.432	1.00	36.19
ATOM	502	CA	ILE	221	64.563	49.305	18.394	1.00	36.77
ATOM	503	CB	ILE	221	65.756	48.996	17.457	1.00	34.41
ATOM	504	CG2	ILE	221	66.270	50.276	16.814	1.00	38.54
ATOM	505	CG1	ILE	221	66.864	48.267	18.221	1.00	32.93
ATOM	506	CD1	ILE	221	67.984	47.752	17.338	1.00	31.12
ATOM	507	C	ILE	221	64.002	47.971	18.888	1.00	38.22
ATOM	508	O	ILE	221	63.499	47.181	18.089	1.00	38.90
ATOM	509	N	ILE	222	64.048	47.719	20.191	1.00	35.75
ATOM	510	CA	ILE	222	63.557	46.446	20.702	1.00	31.77
ATOM	511	CB	ILE	222	64.086	46.152	22.130	1.00	33.14
ATOM	512	CG2	ILE	222	63.203	46.813	23.183	1.00	24.60
ATOM	513	CG1	ILE	222	64.147	44.638	22.350	1.00	32.60
ATOM	514	CD1	ILE	222	64.860	44.226	23.609	1.00	34.52
ATOM	515	C	ILE	222	62.042	46.240	20.624	1.00	32.56
ATOM	516	O	ILE	222	61.581	45.109	20.452	1.00	35.74
ATOM	517	N	THR	223	61.262	47.313	20.720	1.00	29.43
ATOM	518	CA	THR	223	59.806	47.170	20.651	1.00	33.57
ATOM	519	CB	THR	223	59.075	48.514	20.903	1.00	38.99
ATOM	520	OG1	THR	223					



ATOM	522	C	THR	223	59.355	46.528	19.325	1.00	31.45
ATOM	523	O	THR	223	58.571	45.571	19.334	1.00	26.77
ATOM	524	N	PRO	224	59.824	47.054	18.173	1.00	31.35
ATOM	525	CD	PRO	224	60.570	48.306	17.950	1.00	30.11
ATOM	526	CA	PRO	224	59.424	46.462	16.891	1.00	30.38
ATOM	527	CB	PRO	224	60.149	47.336	15.865	1.00	30.09
ATOM	528	CG	PRO	224	60.200	48.659	16.530	1.00	31.86
ATOM	529	C	PRO	224	59.882	45.007	16.795	1.00	29.51
ATOM	530	O	PRO	224	59.147	44.153	16.295	1.00	32.52
ATOM	531	N	ALA	225	61.090	44.734	17.285	1.00	22.63
ATOM	532	CA	ALA	225	61.650	43.385	17.268	1.00	20.88
ATOM	533	CB	ALA	225	63.046	43.386	17.862	1.00	20.57
ATOM	534	C	ALA	225	60.752	42.416	18.026	1.00	23.53
ATOM	535	O	ALA	225	60.455	41.323	17.544	1.00	25.07
ATOM	536	N	ILE	226	60.296	42.828	19.202	1.00	22.61
ATOM	537	CA	ILE	226	59.420	41.989	20.007	1.00	19.46
ATOM	538	CB	ILE	226	59.120	42.644	21.360	1.00	20.25
ATOM	539	CG2	ILE	226	58.071	41.843	22.105	1.00	16.75
ATOM	540	CG1	ILE	226	60.401	42.772	22.182	1.00	19.30
ATOM	541	CD1	ILE	226	60.240	43.645	23.413	1.00	20.92
ATOM	542	C	ILE	226	58.112	41.768	19.251	1.00	21.28
ATOM	543	O	ILE	226	57.553	40.670	19.256	1.00	23.75
ATOM	544	N	THR	227	57.629	42.821	18.598	1.00	24.46
ATOM	545	CA	THR	227	56.393	42.752	17.826	1.00	25.81
ATOM	546	CB	THR	227	56.020	44.136	17.260	1.00	31.00
ATOM	547	OG1	THR	227	55.772	45.039	18.345	1.00	35.43
ATOM	548	CG2	THR	227	54.776	44.049	16.388	1.00	29.01
ATOM	549	C	THR	227	56.508	41.728	16.691	1.00	22.85
ATOM	550	O	THR	227	55.589	40.939	16.469	1.00	22.84
ATOM	551	N	ARG	228	57.647	41.713	16.004	1.00	16.09
ATOM	552	CA	ARG	228	57.862	40.765	14.919	1.00	16.97
ATOM	553	CB	ARG	228	59.161	41.064	14.174	1.00	14.71
ATOM	554	CG	ARG	228	59.137	42.369	13.391	1.00	16.22
ATOM	555	CD	ARG	228	60.309	42.447	12.422	1.00	20.90
ATOM	556	NE	ARG	228	61.595	42.207	13.078	1.00	24.94
ATOM	557	CZ	ARG	228	62.243	43.113	13.805	1.00	35.06
ATOM	558	NH1	ARG	228	61.729	44.328	13.973	1.00	36.35
ATOM	559	NH2	ARG	228	63.404	42.807	14.370	1.00	32.78
ATOM	560	C	ARG	228	57.866	39.326	15.431	1.00	21.63
ATOM	561	O	ARG	228	57.477	38.407	14.704	1.00	24.47
ATOM	562	N	VAL	229	58.304	39.128	16.675	1.00	20.00
ATOM	563	CA	VAL	229	58.319	37.793	17.266	1.00	18.39
ATOM	564	CB	VAL	229	59.103	37.745	18.606	1.00	19.20
ATOM	565	CG1	VAL	229	58.938	36.382	19.265	1.00	14.19
ATOM	566	CG2	VAL	229	60.581	38.001	18.356	1.00	14.81
ATOM	567	C	VAL	229	56.875	37.36			

ATOM	569	N	VAL	230	56.058	38.291	18.003	1.00	19.60
ATOM	570	CA	VAL	230	54.651	37.996	18.247	1.00	18.72
ATOM	571	CB	VAL	230	53.930	39.185	18.912	1.00	22.15
ATOM	572	CG1	VAL	230	52.452	38.862	19.113	1.00	15.66
ATOM	573	CG2	VAL	230	54.592	39.522	20.248	1.00	21.05
ATOM	574	C <sup>-</sup>	VAL	230	53.967	37.660	16.917	1.00	26.17
ATOM	575	O	VAL	230	53.188	36.704	16.836	1.00	28.01
ATOM	576	N	ASP	231	54.288	38.426	15.873	1.00	25.07
ATOM	577	CA	ASP	231	53.714	38.216	14.542	1.00	26.10
ATOM	578	CB	ASP	231	54.169	39.309	13.568	1.00	22.15
ATOM	579	CG	ASP	231	53.620	40.684	13.921	1.00	29.49
ATOM	580	OD1	ASP	231	52.587	40.767	14.624	1.00	30.93
ATOM	581	OD2	ASP	231	54.223	41.687	13.481	1.00	31.74
ATOM	582	C	ASP	231	54.087	36.842	13.989	1.00	27.35
ATOM	583	O	ASP	231	53.245	36.154	13.408	1.00	25.89
ATOM	584	N	PHE	232	55.347	36.451	14.175	1.00	24.29
ATOM	585	CA	PHE	232	55.825	35.154	13.714	1.00	22.90
ATOM	586	CB	PHE	232	57.302	34.956	14.090	1.00	20.56
ATOM	587	CG	PHE	232	57.762	33.525	14.007	1.00	24.20
ATOM	588	CD1	PHE	232	57.952	32.910	12.772	1.00	23.44
ATOM	589	CD2	PHE	232	57.959	32.776	15.167	1.00	19.41
ATOM	590	CE1	PHE	232	58.329	31.567	12.689	1.00	19.53
ATOM	591	CE2	PHE	232	58.336	31.431	15.100	1.00	21.09
ATOM	592	CZ	PHE	232	58.520	30.824	13.858	1.00	21.61
ATOM	593	C	PHE	232	54.984	34.047	14.341	1.00	24.18
ATOM	594	O	PHE	232	54.481	33.160	13.645	1.00	22.26
ATOM	595	N	ALA	233	54.810	34.127	15.656	1.00	23.90
ATOM	596	CA	ALA	233	54.048	33.128	16.397	1.00	22.60
ATOM	597	CB	ALA	233	54.088	33.435	17.890	1.00	15.34
ATOM	598	C	ALA	233	52.609	33.040	15.917	1.00	22.04
ATOM	599	O	ALA	233	52.084	31.948	15.697	1.00	22.86
ATOM	600	N	LYS	234	51.978	34.195	15.743	1.00	25.04
ATOM	601	CA	LYS	234	50.593	34.248	15.298	1.00	27.68
ATOM	602	CB	LYS	234	50.096	35.691	15.292	1.00	31.41
ATOM	603	CG	LYS	234	49.845	36.248	16.682	1.00	40.37
ATOM	604	CD	LYS	234	49.212	37.626	16.604	1.00	57.53
ATOM	605	CE	LYS	234	48.772	38.112	17.974	1.00	64.28
ATOM	606	NZ	LYS	234	48.164	39.473	17.904	1.00	67.19
ATOM	607	C	LYS	234	50.358	33.588	13.939	1.00	26.42
ATOM	608	O	LYS	234	49.269	33.067	13.674	1.00	31.34
ATOM	609	N	LYS	235	51.382	33.588	13.093	1.00	24.38
ATOM	610	CA	LYS	235	51.278	32.985	11.770	1.00	26.42
ATOM	611	CB	LYS	235	52.244	33.664	10.805	1.00	24.92
ATOM	612	CG	LYS	235	51.908	35.127	10.583	1.00	22.41
ATOM	613	CD	LYS	235	52.843	35.775	9.588	1.00	29.38
ATOM	614	CE	LYS	235					



ATOM	616	C	LYS	235	51.470	31.469	11.759	1.00	30.02
ATOM	617	O	LYS	235	51.417	30.838	10.699	1.00	30.37
ATOM	618	N	LEU	236	51.722	30.889	12.930	1.00	32.39
ATOM	619	CA	LEU	236	51.878	29.443	13.053	1.00	36.24
ATOM	620	CB	LEU	236	52.944	29.080	14.089	1.00	29.91
ATOM	621	CG	LEU	236	54.373	29.516	13.765	1.00	24.69
ATOM	622	CD1	LEU	236	55.299	29.054	14.877	1.00	22.71
ATOM	623	CD2	LEU	236	54.811	28.942	12.427	1.00	24.48
ATOM	624	C	LEU	236	50.520	28.891	13.470	1.00	41.22
ATOM	625	O	LEU	236	49.936	29.333	14.467	1.00	41.45
ATOM	626	N	PRO	237	50.012	27.895	12.729	1.00	47.86
ATOM	627	CD	PRO	237	50.739	27.190	11.657	1.00	49.32
ATOM	628	CA	PRO	237	48.713	27.262	12.992	1.00	50.28
ATOM	629	CB	PRO	237	48.669	26.128	11.962	1.00	55.25
ATOM	630	CG	PRO	237	50.135	25.818	11.706	1.00	54.08
ATOM	631	C	PRO	237	48.495	26.751	14.422	1.00	47.94
ATOM	632	O	PRO	237	47.533	27.134	15.087	1.00	42.48
ATOM	633	N	MET	238	49.415	25.927	14.906	1.00	49.51
ATOM	634	CA	MET	238	49.306	25.354	16.245	1.00	53.49
ATOM	635	CB	MET	238	50.379	24.275	16.424	1.00	52.52
ATOM	636	CG	MET	238	50.028	22.959	15.728	1.00	56.00
ATOM	637	SD	MET	238	51.443	21.961	15.204	1.00	50.16
ATOM	638	CE	MET	238	50.896	21.440	13.552	1.00	55.71
ATOM	639	C	MET	238	49.352	26.362	17.395	1.00	54.20
ATOM	640	O	MET	238	48.930	26.058	18.515	1.00	54.72
ATOM	641	N	PHE	239	49.803	27.578	17.101	1.00	50.11
ATOM	642	CA	PHE	239	49.917	28.619	18.117	1.00	41.11
ATOM	643	CB	PHE	239	51.089	29.552	17.788	1.00	34.80
ATOM	644	CG	PHE	239	51.336	30.607	18.826	1.00	30.25
ATOM	645	CD1	PHE	239	52.127	30.332	19.937	1.00	25.66
ATOM	646	CD2	PHE	239	50.786	31.878	18.690	1.00	26.30
ATOM	647	CE1	PHE	239	52.368	31.307	20.896	1.00	30.28
ATOM	648	CE2	PHE	239	51.019	32.862	19.644	1.00	30.49
ATOM	649	CZ	PHE	239	51.813	32.576	20.750	1.00	29.00
ATOM	650	C	PHE	239	48.647	29.434	18.337	1.00	35.65
ATOM	651	O	PHE	239	48.151	29.521	19.457	1.00	30.27
ATOM	652	N	SER	240	48.133	30.037	17.272	1.00	36.49
ATOM	653	CA	SER	240	46.936	30.866	17.359	1.00	36.37
ATOM	654	CB	SER	240	46.622	31.466	15.994	1.00	35.87
ATOM	655	C	SER	240	45.707	30.145	17.936	1.00	40.37
ATOM	656	O	SER	240	44.784	30.789	18.438	1.00	37.47
ATOM	657	N	GLU	241	45.713	28.814	17.889	1.00	43.00
ATOM	658	CA	GLU	241	44.605	28.004	18.404	1.00	46.31
ATOM	659	CB	GLU	241	44.714	26.566	17.881	1.00	55.84
ATOM	660	CG	GLU	241	44.750	26.422	16.360	1.00	69.03
ATOM	661	CD	GLU	241	45.				

ATOM	663	OE2	GLU	241	44.765	24.629	14.770	1.00	70.58
ATOM	664	C	GLU	241	44.587	27.961	19.933	1.00	42.60
ATOM	665	O	GLU	241	43.541	27.740	20.545	1.00	43.23
ATOM	666	N	LEU	242	45.762	28.125	20.535	1.00	39.31
ATOM	667	CA	LEU	242	45.926	28.086	21.987	1.00	34.54
ATOM	668	CB	LEU	242	47.417	28.109	22.344	1.00	28.35
ATOM	669	CG	LEU	242	48.311	26.974	21.853	1.00	27.59
ATOM	670	CD1	LEU	242	49.750	27.307	22.180	1.00	20.72
ATOM	671	CD2	LEU	242	47.902	25.661	22.500	1.00	24.97
ATOM	672	C	LEU	242	45.242	29.240	22.711	1.00	32.23
ATOM	673	O	LEU	242	44.956	30.282	22.119	1.00	31.50
ATOM	674	N	PRO	243	44.954	29.060	24.010	1.00	34.39
ATOM	675	CD	PRO	243	45.118	27.843	24.827	1.00	31.68
ATOM	676	CA	PRO	243	44.309	30.134	24.773	1.00	34.39
ATOM	677	CB	PRO	243	44.092	29.498	26.154	1.00	32.34
ATOM	678	CG	PRO	243	44.081	28.026	25.892	1.00	33.80
ATOM	679	C	PRO	243	45.300	31.303	24.873	1.00	35.56
ATOM	680	O	PRO	243	46.517	31.082	24.897	1.00	34.99
ATOM	681	N	CYS	244	44.791	32.532	24.946	1.00	34.23
ATOM	682	CA	CYS	244	45.648	33.714	25.062	1.00	37.03
ATOM	683	CB	CYS	244	44.820	34.960	25.376	1.00	43.49
ATOM	684	SG	CYS	244	43.820	35.531	24.007	1.00	71.28
ATOM	685	C	CYS	244	46.716	33.555	26.135	1.00	34.99
ATOM	686	O	CYS	244	47.894	33.802	25.882	1.00	37.49
ATOM	687	N	GLU	245	46.305	33.125	27.326	1.00	33.03
ATOM	688	CA	GLU	245	47.249	32.944	28.424	1.00	35.72
ATOM	689	CB	GLU	245	46.559	32.469	29.716	1.00	37.85
ATOM	690	CG	GLU	245	45.294	31.633	29.549	1.00	46.81
ATOM	691	CD	GLU	245	44.029	32.478	29.480	1.00	44.81
ATOM	692	OE1	GLU	245	43.606	33.012	30.527	1.00	33.05
ATOM	693	OE2	GLU	245	43.454	32.599	28.377	1.00	48.22
ATOM	694	C	GLU	245	48.414	32.035	28.047	1.00	32.29
ATOM	695	O	GLU	245	49.558	32.319	28.399	1.00	35.92
ATOM	696	N	ASP	246	48.134	30.975	27.295	1.00	30.64
ATOM	697	CA	ASP	246	49.182	30.058	26.855	1.00	28.23
ATOM	698	CB	ASP	246	48.575	28.809	26.208	1.00	30.51
ATOM	699	CG	ASP	246	48.213	27.737	27.222	1.00	33.18
ATOM	700	OD1	ASP	246	48.265	28.006	28.439	1.00	31.26
ATOM	701	OD2	ASP	246	47.884	26.613	26.796	1.00	33.85
ATOM	702	C	ASP	246	50.104	30.757	25.860	1.00	30.10
ATOM	703	O	ASP	246	51.330	30.651	25.950	1.00	27.08
ATOM	704	N	GLN	247	49.500	31.477	24.918	1.00	30.39
ATOM	705	CA	GLN	247	50.249	32.208	23.901	1.00	29.08
ATOM	706	CB	GLN	247	49.295	32.949	22.964	1.00	27.34
ATOM	707	CG	GLN	247	48.390	32.034	22.147	1.00	28.95
ATOM	708	CD	GLN						

ATOM	710	NE2	GLN	247	46.439	32.185	20.729	1.00	35.19
ATOM	711	C	GLN	247	51.190	33.196	24.575	1.00	27.51
ATOM	712	O	GLN	247	52.377	33.261	24.256	1.00	28.70
ATOM	713	N	ILE	248	50.661	33.921	25.552	1.00	27.81
ATOM	714	CA	ILE	248	51.431	34.908	26.295	1.00	29.41
ATOM	715	CB	ILE	248	50.525	35.662	27.303	1.00	28.96
ATOM	716	CG2	ILE	248	51.356	36.476	28.279	1.00	28.67
ATOM	717	CG1	ILE	248	49.555	36.571	26.543	1.00	28.83
ATOM	718	CD1	ILE	248	48.514	37.236	27.420	1.00	30.76
ATOM	719	C	ILE	248	52.618	34.259	27.006	1.00	28.39
ATOM	720	O	ILE	248	53.759	34.715	26.869	1.00	27.88
ATOM	721	N	ILE	249	52.356	33.177	27.732	1.00	26.07
ATOM	722	CA	ILE	249	53.413	32.474	28.454	1.00	27.37
ATOM	723	CB	ILE	249	52.839	31.294	29.281	1.00	30.32
ATOM	724	CG2	ILE	249	53.958	30.425	29.840	1.00	31.29
ATOM	725	CG1	ILE	249	51.987	31.831	30.429	1.00	30.31
ATOM	726	CD1	ILE	249	51.295	30.753	31.230	1.00	31.30
ATOM	727	C	ILE	249	54.510	31.974	27.509	1.00	28.63
ATOM	728	O	ILE	249	55.701	32.100	27.808	1.00	29.59
ATOM	729	N	LEU	250	54.110	31.442	26.357	1.00	29.03
ATOM	730	CA	LEU	250	55.068	30.934	25.380	1.00	22.44
ATOM	731	CB	LEU	250	54.351	30.166	24.266	1.00	24.30
ATOM	732	CG	LEU	250	53.665	28.866	24.687	1.00	23.20
ATOM	733	CD1	LEU	250	52.951	28.273	23.502	1.00	20.36
ATOM	734	CD2	LEU	250	54.685	27.880	25.238	1.00	19.45
ATOM	735	C	LEU	250	55.919	32.055	24.794	1.00	18.97
ATOM	736	O	LEU	250	57.133	31.903	24.648	1.00	18.37
ATOM	737	N	LEU	251	55.291	33.180	24.468	1.00	20.63
ATOM	738	CA	LEU	251	56.026	34.318	23.915	1.00	27.43
ATOM	739	CB	LEU	251	55.065	35.412	23.449	1.00	22.92
ATOM	740	CG	LEU	251	54.364	35.093	22.128	1.00	24.72
ATOM	741	CD1	LEU	251	53.342	36.167	21.821	1.00	32.13
ATOM	742	CD2	LEU	251	55.389	34.981	21.009	1.00	22.46
ATOM	743	C	LEU	251	57.026	34.875	24.930	1.00	27.23
ATOM	744	O	LEU	251	58.202	35.078	24.614	1.00	26.48
ATOM	745	N	LYS	252	56.561	35.094	26.156	1.00	27.34
ATOM	746	CA	LYS	252	57.425	35.598	27.215	1.00	28.95
ATOM	747	CB	LYS	252	56.649	35.715	28.527	1.00	32.89
ATOM	748	CG	LYS	252	55.570	36.783	28.530	1.00	35.06
ATOM	749	CD	LYS	252	55.084	37.028	29.943	1.00	42.82
ATOM	750	CE	LYS	252	54.124	38.191	30.003	1.00	53.05
ATOM	751	NZ	LYS	252	53.677	38.451	31.398	1.00	64.03
ATOM	752	C	LYS	252	58.605	34.647	27.405	1.00	27.66
ATOM	753	O	LYS	252	59.734	35.076	27.646	1.00	33.16
ATOM	754	N	GLY	253	58.344	33.357	27.243	1.00	24.50
ATOM	755	CA							





ATOM	804	CA	SER	260	69.056	36.324	19.947	1.00	16.90
ATOM	805	CB	SER	260	69.434	35.631	21.251	1.00	15.56
ATOM	806	OG	SER	260	69.093	36.455	22.352	1.00	22.98
ATOM	807	C	SER	260	69.471	35.487	18.746	1.00	14.52
ATOM	808	O	SER	260	70.496	35.761	18.129	1.00	22.82
ATOM	809	N-	LEU	261	68.663	34.490	18.397	1.00	16.50
ATOM	810	CA	LEU	261	68.948	33.642	17.241	1.00	17.78
ATOM	811	CB	LEU	261	67.878	32.552	17.092	1.00	18.38
ATOM	812	CG	LEU	261	67.890	31.708	15.812	1.00	14.47
ATOM	813	CD1	LEU	261	69.159	30.877	15.728	1.00	16.76
ATOM	814	CD2	LEU	261	66.672	30.806	15.793	1.00	14.06
ATOM	815	C	LEU	261	68.959	34.519	15.992	1.00	20.40
ATOM	816	O	LEU	261	69.885	34.450	15.181	1.00	22.00
ATOM	817	N	ARG	262	67.934	35.356	15.854	1.00	21.02
ATOM	818	CA	ARG	262	67.821	36.249	14.705	1.00	22.84
ATOM	819	CB	ARG	262	66.530	37.067	14.782	1.00	20.29
ATOM	820	CG	ARG	262	65.311	36.267	14.364	1.00	23.33
ATOM	821	CD	ARG	262	64.007	37.026	14.509	1.00	19.05
ATOM	822	NE	ARG	262	62.959	36.321	13.775	1.00	21.32
ATOM	823	CZ	ARG	262	61.780	36.837	13.441	1.00	23.44
ATOM	824	NH1	ARG	262	61.465	38.081	13.780	1.00	22.99
ATOM	825	NH2	ARG	262	60.933	36.116	12.713	1.00	22.09
ATOM	826	C	ARG	262	69.035	37.154	14.561	1.00	22.66
ATOM	827	O	ARG	262	69.434	37.483	13.445	1.00	22.41
ATOM	828	N	ALA	263	69.625	37.545	15.689	1.00	23.52
ATOM	829	CA	ALA	263	70.820	38.386	15.677	1.00	22.37
ATOM	830	CB	ALA	263	70.986	39.089	17.018	1.00	22.76
ATOM	831	C	ALA	263	72.052	37.530	15.366	1.00	22.85
ATOM	832	O	ALA	263	72.882	37.897	14.529	1.00	25.50
ATOM	833	N	ALA	264	72.131	36.365	16.005	1.00	21.68
ATOM	834	CA	ALA	264	73.242	35.438	15.826	1.00	20.26
ATOM	835	CB	ALA	264	73.092	34.256	16.763	1.00	15.97
ATOM	836	C	ALA	264	73.401	34.957	14.382	1.00	23.11
ATOM	837	O	ALA	264	74.523	34.831	13.892	1.00	24.87
ATOM	838	N	VAL	265	72.293	34.679	13.697	1.00	22.94
ATOM	839	CA	VAL	265	72.380	34.226	12.306	1.00	28.98
ATOM	840	CB	VAL	265	71.072	33.547	11.797	1.00	25.97
ATOM	841	CG1	VAL	265	70.751	32.330	12.638	1.00	26.27
ATOM	842	CG2	VAL	265	69.907	34.527	11.797	1.00	26.64
ATOM	843	C	VAL	265	72.761	35.373	11.369	1.00	28.81
ATOM	844	O	VAL	265	72.966	35.160	10.176	1.00	31.92
ATOM	845	N	ARG	266	72.830	36.587	11.915	1.00	31.83
ATOM	846	CA	ARG	266	73.210	37.774	11.150	1.00	33.19
ATOM	847	CB	ARG	266	72.141	38.861	11.258	1.00	31.67
ATOM	848	CG	ARG	266	70.986	38.623	10.320	1.00	26.82
ATOM	849	CD	ARG	266	69.913				



ATOM	851	CZ	ARG	266	67.688	39.927	9.410	1.00	37.39
ATOM	852	NH1	ARG	266	67.198	40.491	10.509	1.00	29.92
ATOM	853	NH2	ARG	266	66.918	39.770	8.340	1.00	31.24
ATOM	854	C	ARG	266	74.565	38.307	11.604	1.00	36.31
ATOM	855	O	ARG	266	74.821	39.516	11.575	1.00	38.56
ATOM	856	N-	TYR	267	75.416	37.393	12.056	1.00	34.21
ATOM	857	CA	TYR	267	76.755	37.733	12.502	1.00	35.24
ATOM	858	CB	TYR	267	77.283	36.640	13.440	1.00	32.37
ATOM	859	CG	TYR	267	78.774	36.699	13.703	1.00	35.07
ATOM	860	CD1	TYR	267	79.303	37.555	14.669	1.00	33.94
ATOM	861	CE1	TYR	267	80.677	37.609	14.905	1.00	36.60
ATOM	862	CD2	TYR	267	79.658	35.894	12.979	1.00	34.68
ATOM	863	CE2	TYR	267	81.029	35.940	13.208	1.00	36.07
ATOM	864	CZ	TYR	267	81.533	36.797	14.170	1.00	37.14
ATOM	865	OH	TYR	267	82.889	36.835	14.396	1.00	41.52
ATOM	866	C	TYR	267	77.639	37.831	11.263	1.00	37.68
ATOM	867	O	TYR	267	77.609	36.943	10.410	1.00	36.48
ATOM	868	N	ASP	268	78.400	38.915	11.150	1.00	39.58
ATOM	869	CA	ASP	268	79.301	39.096	10.016	1.00	42.77
ATOM	870	CB	ASP	268	79.170	40.511	9.434	1.00	44.38
ATOM	871	CG	ASP	268	80.145	40.770	8.290	1.00	50.31
ATOM	872	OD1	ASP	268	80.290	39.901	7.400	1.00	55.79
ATOM	873	OD2	ASP	268	80.773	41.847	8.280	1.00	50.24
ATOM	874	C	ASP	268	80.737	38.846	10.466	1.00	42.51
ATOM	875	O	ASP	268	81.305	39.645	11.208	1.00	42.75
ATOM	876	N	PRO	269	81.346	37.733	10.020	1.00	44.56
ATOM	877	CD	PRO	269	80.770	36.697	9.146	1.00	42.66
ATOM	878	CA	PRO	269	82.725	37.395	10.393	1.00	45.98
ATOM	879	CB	PRO	269	82.991	36.111	9.607	1.00	44.04
ATOM	880	CG	PRO	269	81.631	35.506	9.458	1.00	43.33
ATOM	881	C	PRO	269	83.710	38.492	10.004	1.00	50.31
ATOM	882	O	PRO	269	84.630	38.800	10.761	1.00	49.83
ATOM	883	N	ALA	270	83.486	39.100	8.840	1.00	53.62
ATOM	884	CA	ALA	270	84.348	40.165	8.329	1.00	54.54
ATOM	885	CB	ALA	270	83.892	40.585	6.929	1.00	51.24
ATOM	886	C	ALA	270	84.449	41.389	9.248	1.00	55.69
ATOM	887	O	ALA	270	85.488	42.045	9.294	1.00	57.92
ATOM	888	N	SER	271	83.384	41.685	9.989	1.00	54.71
ATOM	889	CA	SER	271	83.378	42.838	10.889	1.00	51.26
ATOM	890	CB	SER	271	82.182	43.740	10.575	1.00	49.92
ATOM	891	OG	SER	271	82.065	43.976	9.183	1.00	60.09
ATOM	892	C	SER	271	83.305	42.443	12.360	1.00	50.78
ATOM	893	O	SER	271	83.482	43.288	13.240	1.00	52.11
ATOM	894	N	ASP	272	83.051	41.162	12.619	1.00	48.96
ATOM	895	CA	ASP	272	82.898	40.643	13.978	1.00	45.53
ATOM	896	CB	ASP	272	84.206	40.765	14.776	1.00	44.82
ATOM	897	CG	ASP	272	84.142	40.064	16.131	1.00	47.66

ATOM	898	OD1 ASP	272	84.750	40.581	17.091	1.00	48.64
ATOM	899	OD2 ASP	272	83.495	38.999	16.238	1.00	43.85
ATOM	900	C ASP	272	81.765	41.437	14.636	1.00	44.46
ATOM	901	O ASP	272	81.904	41.958	15.747	1.00	42.41
ATOM	902	N THR	273	80.652	41.551	13.915	1.00	39.79
ATOM	903	CA THR	273	79.492	42.282	14.401	1.00	38.82
ATOM	904	CB THR	273	79.334	43.648	13.670	1.00	39.73
ATOM	905	OG1 THR	273	79.288	43.439	12.254	1.00	39.36
ATOM	906	CG2 THR	273	80.496	44.578	13.991	1.00	41.31
ATOM	907	C THR	273	78.203	41.485	14.211	1.00	38.36
ATOM	908	O THR	273	78.151	40.546	13.408	1.00	33.79
ATOM	909	N LEU	274	77.187	41.835	14.995	1.00	36.91
ATOM	910	CA LEU	274	75.869	41.212	14.912	1.00	34.49
ATOM	911	CB LEU	274	75.342	40.822	16.297	1.00	30.37
ATOM	912	CG LEU	274	75.948	39.651	17.069	1.00	32.97
ATOM	913	CD1 LEU	274	75.297	39.593	18.440	1.00	28.23
ATOM	914	CD2 LEU	274	75.749	38.341	16.318	1.00	26.86
ATOM	915	C LEU	274	74.956	42.289	14.352	1.00	35.35
ATOM	916	O LEU	274	75.171	43.478	14.601	1.00	37.47
ATOM	917	N THR	275	73.942	41.890	13.599	1.00	34.05
ATOM	918	CA THR	275	73.020	42.868	13.052	1.00	32.62
ATOM	919	CB THR	275	72.824	42.674	11.542	1.00	35.14
ATOM	920	OG1 THR	275	74.108	42.590	10.909	1.00	39.50
ATOM	921	CG2 THR	275	72.064	43.851	10.952	1.00	30.94
ATOM	922	C THR	275	71.699	42.746	13.793	1.00	30.92
ATOM	923	O THR	275	71.100	41.670	13.845	1.00	36.53
ATOM	924	N LEU	276	71.291	43.835	14.434	1.00	28.10
ATOM	925	CA LEU	276	70.051	43.868	15.192	1.00	27.78
ATOM	926	CB LEU	276	70.205	44.780	16.420	1.00	22.51
ATOM	927	CG LEU	276	71.383	44.532	17.373	1.00	25.89
ATOM	928	CD1 LEU	276	71.225	45.408	18.608	1.00	20.70
ATOM	929	CD2 LEU	276	71.456	43.069	17.782	1.00	20.79
ATOM	930	C LEU	276	68.930	44.376	14.296	1.00	27.27
ATOM	931	O LEU	276	69.068	45.430	13.672	1.00	29.06
ATOM	932	N SER	277	67.854	43.598	14.187	1.00	25.97
ATOM	933	CA SER	277	66.697	43.957	13.366	1.00	28.63
ATOM	934	CB SER	277	65.990	45.177	13.967	1.00	27.78
ATOM	935	OG SER	277	65.561	44.905	15.290	1.00	22.65
ATOM	936	C SER	277	67.067	44.209	11.897	1.00	30.31
ATOM	937	O SER	277	66.374	44.939	11.181	1.00	28.52
ATOM	938	N GLY	278	68.168	43.597	11.465	1.00	31.24
ATOM	939	CA GLY	278	68.638	43.754	10.101	1.00	39.59
ATOM	940	C GLY	278	68.999	45.178	9.706	1.00	44.55
ATOM	941	O GLY	278	69.104	45.479	8.517	1.00	46.66
ATOM	942	N GLU	279	69.234	46.046	10.686	1.00	43.47
ATOM	943	CA GLU	279	69.566	47.435	10.387	1.00	43.87
ATOM	944	CB GLU	279	68.314	48.312	10.515	1.00	44.28

ATOM	945	CG	GLU	279	67.703	48.322	11.908	1.00	52.30
ATOM	946	CD	GLU	279	66.440	49.159	12.001	1.00	60.23
ATOM	947	OE1	GLU	279	66.398	50.074	12.853	1.00	63.06
ATOM	948	OE2	GLU	279	65.485	48.894	11.238	1.00	65.67
ATOM	949	C	GLU	279	70.700	48.038	11.216	1.00	42.40
ATOM	950	O	GLU	279	71.330	49.001	10.787	1.00	43.89
ATOM	951	N	MET	280	70.977	47.472	12.388	1.00	40.86
ATOM	952	CA	MET	280	72.027	48.009	13.248	1.00	32.80
ATOM	953	CB	MET	280	71.435	48.415	14.603	1.00	29.25
ATOM	954	CG	MET	280	72.384	49.193	15.506	1.00	31.64
ATOM	955	SD	MET	280	71.830	49.235	17.232	1.00	34.02
ATOM	956	CE	MET	280	70.566	50.495	17.197	1.00	26.56
ATOM	957	C	MET	280	73.172	47.033	13.465	1.00	32.77
ATOM	958	O	MET	280	72.983	45.971	14.058	1.00	34.61
ATOM	959	N	ALA	281	74.351	47.375	12.959	1.00	31.87
ATOM	960	CA	ALA	281	75.523	46.526	13.147	1.00	34.71
ATOM	961	CB	ALA	281	76.519	46.727	12.023	1.00	34.42
ATOM	962	C	ALA	281	76.125	46.950	14.482	1.00	36.76
ATOM	963	O	ALA	281	76.416	48.129	14.693	1.00	34.59
ATOM	964	N	VAL	282	76.275	45.993	15.390	1.00	37.16
ATOM	965	CA	VAL	282	76.798	46.263	16.721	1.00	37.83
ATOM	966	CB	VAL	282	75.692	46.023	17.780	1.00	37.58
ATOM	967	CG1	VAL	282	76.219	46.271	19.175	1.00	48.99
ATOM	968	CG2	VAL	282	74.514	46.939	17.514	1.00	43.59
ATOM	969	C	VAL	282	78.017	45.400	17.046	1.00	39.04
ATOM	970	O	VAL	282	78.081	44.230	16.660	1.00	39.16
ATOM	971	N	LYS	283	78.989	45.993	17.735	1.00	38.75
ATOM	972	CA	LYS	283	80.205	45.287	18.136	1.00	42.18
ATOM	973	CB	LYS	283	81.428	46.208	18.045	1.00	47.46
ATOM	974	CG	LYS	283	81.803	46.617	16.632	1.00	51.71
ATOM	975	CD	LYS	283	83.092	47.416	16.618	1.00	59.26
ATOM	976	CE	LYS	283	83.481	47.813	15.202	1.00	62.52
ATOM	977	NZ	LYS	283	82.492	48.742	14.588	1.00	66.27
ATOM	978	C	LYS	283	80.075	44.746	19.559	1.00	38.78
ATOM	979	O	LYS	283	79.283	45.257	20.356	1.00	40.63
ATOM	980	N	ARG	284	80.900	43.753	19.881	1.00	36.01
ATOM	981	CA	ARG	284	80.908	43.104	21.189	1.00	38.62
ATOM	982	CB	ARG	284	82.150	42.224	21.327	1.00	38.83
ATOM	983	CG	ARG	284	82.220	41.091	20.333	1.00	41.87
ATOM	984	CD	ARG	284	83.521	40.335	20.451	1.00	39.60
ATOM	985	NE	ARG	284	83.506	39.120	19.644	1.00	45.18
ATOM	986	CZ	ARG	284	83.259	37.905	20.128	1.00	44.79
ATOM	987	NH1	ARG	284	83.005	37.739	21.421	1.00	41.84
ATOM	988	NH2	ARG	284	83.271	36.852	19.319	1.00	42.27
ATOM	989	C	ARG	284	80.829	44.051	22.385	1.00	41.18
ATOM	990	O	ARG	284	79.995	43.867	23.274	1.00	44.38
ATOM	991	N	GLU	285	81.703	45.052	22.416	1.00	38.71

ATOM	992	CA	GLU	285	81.724	46.002	23.525	1.00	37.18
ATOM	993	CB	GLU	285	82.950	46.906	23.422	1.00	36.65
ATOM	994	C	GLU	285	80.444	46.838	23.614	1.00	35.71
ATOM	995	O	GLU	285	79.921	47.074	24.704	1.00	33.00
ATOM	996	N	GLN	286	79.920	47.245	22.463	1.00	32.01
ATOM	997	CA	GLN	286	78.714	48.061	22.425	1.00	32.31
ATOM	998	CB	GLN	286	78.440	48.525	20.997	1.00	38.24
ATOM	999	CG	GLN	286	79.565	49.352	20.392	1.00	42.42
ATOM	1000	CD	GLN	286	79.277	49.761	18.964	1.00	44.79
ATOM	1001	OE1	GLN	286	79.103	48.910	18.089	1.00	42.21
ATOM	1002	NE2	GLN	286	79.215	51.063	18.719	1.00	47.53
ATOM	1003	C	GLN	286	77.484	47.355	23.002	1.00	33.08
ATOM	1004	O	GLN	286	76.770	47.929	23.827	1.00	30.95
ATOM	1005	N	LEU	287	77.245	46.114	22.579	1.00	31.49
ATOM	1006	CA	LEU	287	76.095	45.350	23.068	1.00	31.01
ATOM	1007	CB	LEU	287	75.892	44.073	22.242	1.00	24.63
ATOM	1008	CG	LEU	287	74.498	43.780	21.661	1.00	27.34
ATOM	1009	CD1	LEU	287	74.382	42.282	21.359	1.00	20.50
ATOM	1010	CD2	LEU	287	73.393	44.205	22.616	1.00	14.41
ATOM	1011	C	LEU	287	76.298	44.986	24.538	1.00	32.80
ATOM	1012	O	LEU	287	75.351	45.014	25.334	1.00	32.10
ATOM	1013	N	LYS	288	77.536	44.641	24.885	1.00	32.54
ATOM	1014	CA	LYS	288	77.897	44.280	26.251	1.00	30.70
ATOM	1015	CB	LYS	288	79.376	43.893	26.315	1.00	31.24
ATOM	1016	CG	LYS	288	79.834	43.382	27.662	1.00	34.69
ATOM	1017	CD	LYS	288	81.227	42.784	27.574	1.00	37.69
ATOM	1018	CE	LYS	288	81.638	42.177	28.904	1.00	42.86
ATOM	1019	NZ	LYS	288	82.883	41.369	28.786	1.00	49.63
ATOM	1020	C	LYS	288	77.611	45.448	27.189	1.00	28.74
ATOM	1021	O	LYS	288	76.827	45.319	28.129	1.00	34.45
ATOM	1022	N	ASN	289	78.190	46.602	26.882	1.00	26.57
ATOM	1023	CA	ASN	289	78.011	47.803	27.691	1.00	30.84
ATOM	1024	CB	ASN	289	79.012	48.879	27.274	1.00	26.04
ATOM	1025	CG	ASN	289	80.437	48.485	27.570	1.00	35.16
ATOM	1026	OD1	ASN	289	80.700	47.718	28.499	1.00	42.54
ATOM	1027	ND2	ASN	289	81.371	48.998	26.784	1.00	32.82
ATOM	1028	C	ASN	289	76.602	48.371	27.620	1.00	35.05
ATOM	1029	O	ASN	289	76.154	49.039	28.550	1.00	36.94
ATOM	1030	N	GLY	290	75.909	48.113	26.515	1.00	32.43
ATOM	1031	CA	GLY	290	74.556	48.614	26.345	1.00	28.66
ATOM	1032	C	GLY	290	73.525	48.024	27.289	1.00	28.48
ATOM	1033	O	GLY	290	72.377	48.467	27.308	1.00	28.17
ATOM	1034	N	GLY	291	73.908	47.002	28.047	1.00	28.66
ATOM	1035	CA	GLY	291	72.969	46.408	28.980	1.00	29.19
ATOM	1036	C	GLY	291	72.976	44.894	29.075	1.	



ATOM	1039	CA	LEU	292	73.410	42.755	28.036	1.00	30.64
ATOM	1040	CB	LEU	292	73.421	42.194	26.611	1.00	27.07
ATOM	1041	CG	LEU	292	72.113	42.348	25.833	1.00	23.27
ATOM	1042	CD1	LEU	292	72.202	41.580	24.532	1.00	22.24
ATOM	1043	CD2	LEU	292	70.950	41.827	26.661	1.00	23.80
ATOM	1044	C <sup>-</sup>	LEU	292	74.530	42.125	28.861	1.00	29.22
ATOM	1045	O	LEU	292	74.365	41.033	29.404	1.00	31.02
ATOM	1046	N	GLY	293	75.671	42.800	28.945	1.00	30.26
ATOM	1047	CA	GLY	293	76.788	42.259	29.700	1.00	28.37
ATOM	1048	C	GLY	293	77.307	40.995	29.040	1.00	29.85
ATOM	1049	O	GLY	293	77.460	40.951	27.820	1.00	32.37
ATOM	1050	N	VAL	294	77.537	39.953	29.832	1.00	30.08
ATOM	1051	CA	VAL	294	78.041	38.687	29.308	1.00	31.62
ATOM	1052	CB	VAL	294	78.466	37.716	30.442	1.00	29.11
ATOM	1053	CG1	VAL	294	79.649	38.292	31.191	1.00	31.37
ATOM	1054	CG2	VAL	294	77.304	37.443	31.396	1.00	26.69
ATOM	1055	C	VAL	294	77.079	37.978	28.351	1.00	32.81
ATOM	1056	O	VAL	294	77.496	37.095	27.591	1.00	33.00
ATOM	1057	N	VAL	295	75.801	38.356	28.380	1.00	30.45
ATOM	1058	CA	VAL	295	74.814	37.752	27.487	1.00	28.02
ATOM	1059	CB	VAL	295	73.378	38.232	27.793	1.00	29.96
ATOM	1060	CG1	VAL	295	72.380	37.575	26.838	1.00	22.55
ATOM	1061	CG2	VAL	295	73.016	37.903	29.232	1.00	20.10
ATOM	1062	C	VAL	295	75.203	38.115	26.057	1.00	29.90
ATOM	1063	O	VAL	295	75.047	37.312	25.140	1.00	34.47
ATOM	1064	N	SER	296	75.762	39.309	25.886	1.00	29.11
ATOM	1065	CA	SER	296	76.215	39.771	24.581	1.00	30.96
ATOM	1066	CB	SER	296	76.785	41.184	24.702	1.00	27.26
ATOM	1067	OG	SER	296	77.300	41.648	23.469	1.00	22.93
ATOM	1068	C	SER	296	77.294	38.811	24.080	1.00	36.41
ATOM	1069	O	SER	296	77.238	38.341	22.939	1.00	38.84
ATOM	1070	N	ASP	297	78.254	38.501	24.954	1.00	35.29
ATOM	1071	CA	ASP	297	79.346	37.585	24.629	1.00	32.14
ATOM	1072	CB	ASP	297	80.245	37.356	25.851	1.00	36.57
ATOM	1073	CG	ASP	297	80.958	38.616	26.307	1.00	41.75
ATOM	1074	OD1	ASP	297	81.492	39.352	25.447	1.00	45.45
ATOM	1075	OD2	ASP	297	80.999	38.861	27.532	1.00	45.15
ATOM	1076	C	ASP	297	78.768	36.249	24.191	1.00	29.61
ATOM	1077	O	ASP	297	79.242	35.644	23.231	1.00	32.90
ATOM	1078	N	ALA	298	77.738	35.804	24.903	1.00	27.85
ATOM	1079	CA	ALA	298	77.071	34.544	24.608	1.00	27.89
ATOM	1080	CB	ALA	298	75.998	34.258	25.657	1.00	21.67
ATOM	1081	C	ALA	298	76.462	34.539	23.202	1.00	28.26
ATOM	1082	O	ALA	298	76.648	33.579	22.446	1.00	30.19
ATOM	1083	N	ILE	299	75.744	35.606	22.853	1.00	25.20</



ATOM	1086	CG2	ILE	299	73.491	36.946	20.078	1.00	22.20
ATOM	1087	CG1	ILE	299	73.145	36.914	22.536	1.00	19.79
ATOM	1088	CD1	ILE	299	72.245	38.139	22.578	1.00	18.33
ATOM	1089	C	ILE	299	76.181	35.752	20.444	1.00	26.28
ATOM	1090	O	ILE	299	76.043	35.095	19.414	1.00	31.72
ATOM	1091	N	PHE	300	77.247	36.512	20.675	1.00	29.35
ATOM	1092	CA	PHE	300	78.338	36.613	19.709	1.00	29.01
ATOM	1093	CB	PHE	300	79.386	37.622	20.182	1.00	29.53
ATOM	1094	CG	PHE	300	79.239	38.978	19.562	1.00	27.60
ATOM	1095	CD1	PHE	300	78.481	39.964	20.179	1.00	24.86
ATOM	1096	CD2	PHE	300	79.853	39.266	18.350	1.00	27.39
ATOM	1097	CE1	PHE	300	78.337	41.218	19.597	1.00	25.66
ATOM	1098	CE2	PHE	300	79.715	40.518	17.761	1.00	25.97
ATOM	1099	CZ	PHE	300	78.956	41.495	18.384	1.00	21.03
ATOM	1100	C	PHE	300	78.988	35.248	19.496	1.00	30.34
ATOM	1101	O	PHE	300	79.309	34.873	18.367	1.00	29.35
ATOM	1102	N	GLU	301	79.181	34.507	20.582	1.00	31.04
ATOM	1103	CA	GLU	301	79.775	33.178	20.499	1.00	33.60
ATOM	1104	CB	GLU	301	80.012	32.607	21.898	1.00	31.64
ATOM	1105	C	GLU	301	78.851	32.265	19.696	1.00	33.90
ATOM	1106	O	GLU	301	79.315	31.473	18.872	1.00	33.33
ATOM	1107	N	LEU	302	77.546	32.386	19.935	1.00	31.13
ATOM	1108	CA	LEU	302	76.556	31.581	19.227	1.00	27.57
ATOM	1109	CB	LEU	302	75.150	31.842	19.776	1.00	25.24
ATOM	1110	CG	LEU	302	73.994	31.131	19.059	1.00	28.59
ATOM	1111	CD1	LEU	302	74.066	29.634	19.299	1.00	25.52
ATOM	1112	CD2	LEU	302	72.660	31.682	19.532	1.00	19.30
ATOM	1113	C	LEU	302	76.601	31.904	17.739	1.00	26.80
ATOM	1114	O	LEU	302	76.682	31.003	16.904	1.00	27.81
ATOM	1115	N	GLY	303	76.576	33.195	17.416	1.00	26.47
ATOM	1116	CA	GLY	303	76.611	33.624	16.030	1.00	26.99
ATOM	1117	C	GLY	303	77.845	33.133	15.295	1.00	33.46
ATOM	1118	O	GLY	303	77.757	32.646	14.164	1.00	32.33
ATOM	1119	N	LYS	304	78.994	33.232	15.956	1.00	34.63
ATOM	1120	CA	LYS	304	80.269	32.813	15.383	1.00	36.20
ATOM	1121	CB	LYS	304	81.399	33.115	16.372	1.00	41.96
ATOM	1122	CG	LYS	304	82.779	33.179	15.757	1.00	47.05
ATOM	1123	CD	LYS	304	83.800	33.610	16.796	1.00	59.47
ATOM	1124	CE	LYS	304	85.179	33.791	16.181	1.00	65.89
ATOM	1125	NZ	LYS	304	85.182	34.863	15.144	1.00	71.01
ATOM	1126	C	LYS	304	80.276	31.332	14.992	1.00	33.17
ATOM	1127	O	LYS	304	80.752	30.974	13.913	1.00	34.44
ATOM	1128	N	SER	305	79.739	30.482	15.861	1.00	31.40
ATOM	1129	CA	SER	305	79.687	29.048	15.594	1.00	33.10
ATOM	1130	CB	SER	305	79.513	28.266	16.900	1	

ATOM	1133	O	SER	305	78.771	27.718	13.816	1.00	35.32
ATOM	1134	N	LEU	306	77.488	29.404	14.580	1.00	32.14
ATOM	1135	CA	LEU	306	76.391	29.121	13.653	1.00	31.02
ATOM	1136	CB	LEU	306	75.138	29.936	13.996	1.00	22.76
ATOM	1137	CG	LEU	306	74.361	29.487	15.235	1.00	24.42
ATOM	1138	CD1	LEU	306	73.094	30.311	15.380	1.00	23.13
ATOM	1139	CD2	LEU	306	74.016	28.009	15.126	1.00	25.53
ATOM	1140	C	LEU	306	76.780	29.354	12.198	1.00	33.11
ATOM	1141	O	LEU	306	76.161	28.796	11.293	1.00	32.60
ATOM	1142	N	SER	307	77.821	30.153	11.975	1.00	36.12
ATOM	1143	CA	SER	307	78.296	30.448	10.624	1.00	38.80
ATOM	1144	CB	SER	307	79.514	31.373	10.677	1.00	41.64
ATOM	1145	OG	SER	307	79.224	32.556	11.401	1.00	54.66
ATOM	1146	C	SER	307	78.650	29.182	9.845	1.00	36.98
ATOM	1147	O	SER	307	78.302	29.055	8.669	1.00	42.87
ATOM	1148	N	ALA	308	79.315	28.239	10.509	1.00	35.72
ATOM	1149	CA	ALA	308	79.719	26.983	9.879	1.00	32.70
ATOM	1150	CB	ALA	308	80.683	26.227	10.782	1.00	33.88
ATOM	1151	C	ALA	308	78.531	26.093	9.521	1.00	34.83
ATOM	1152	O	ALA	308	78.620	25.278	8.600	1.00	39.61
ATOM	1153	N	PHE	309	77.424	26.250	10.244	1.00	31.54
ATOM	1154	CA	PHE	309	76.226	25.453	9.999	1.00	32.43
ATOM	1155	CB	PHE	309	75.259	25.558	11.182	1.00	30.89
ATOM	1156	CG	PHE	309	75.718	24.826	12.415	1.00	33.73
ATOM	1157	CD1	PHE	309	76.769	25.314	13.183	1.00	40.48
ATOM	1158	CD2	PHE	309	75.091	23.654	12.816	1.00	35.96
ATOM	1159	CE1	PHE	309	77.189	24.643	14.334	1.00	37.87
ATOM	1160	CE2	PHE	309	75.502	22.975	13.962	1.00	38.44
ATOM	1161	CZ	PHE	309	76.553	23.471	14.722	1.00	37.34
ATOM	1162	C	PHE	309	75.507	25.809	8.693	1.00	34.76
ATOM	1163	O	PHE	309	74.810	24.969	8.118	1.00	36.18
ATOM	1164	N	ASN	310	75.693	27.040	8.218	1.00	35.80
ATOM	1165	CA	ASN	310	75.060	27.506	6.980	1.00	41.00
ATOM	1166	CB	ASN	310	75.705	26.852	5.755	1.00	51.94
ATOM	1167	CG	ASN	310	77.053	27.452	5.419	1.00	67.92
ATOM	1168	OD1	ASN	310	77.139	28.439	4.687	1.00	77.32
ATOM	1169	ND2	ASN	310	78.116	26.869	5.962	1.00	72.62
ATOM	1170	C	ASN	310	73.560	27.245	6.985	1.00	38.15
ATOM	1171	O	ASN	310	73.034	26.515	6.141	1.00	35.87
ATOM	1172	N	LEU	311	72.885	27.819	7.971	1.00	33.94
ATOM	1173	CA	LEU	311	71.450	27.651	8.111	1.00	32.09
ATOM	1174	CB	LEU	311	71.011	28.009	9.533	1.00	28.06
ATOM	1175	CG	LEU	311	71.656	27.301	10.724	1.00	26.38
ATOM	1176	CD1	LEU	311	71.092	27.883	12.012	1.00	23.56
ATOM	1177	CD2	LEU	311	71.409	25.801	10.651	1.00	21.24
ATOM	1								

ATOM	1180	N	ASP	312	69.569	28.057	6.638	1.00	27.78
ATOM	1181	CA	ASP	312	68.749	28.841	5.733	1.00	27.06
ATOM	1182	CB	ASP	312	68.385	28.049	4.456	1.00	25.84
ATOM	1183	CG	ASP	312	67.580	26.778	4.724	1.00	25.67
ATOM	1184	OD1	ASP	312	67.124	26.541	5.860	1.00	28.20
ATOM	1185	OD2	ASP	312	67.387	26.008	3.762	1.00	27.62
ATOM	1186	C	ASP	312	67.517	29.314	6.514	1.00	28.51
ATOM	1187	O	ASP	312	67.371	28.990	7.703	1.00	25.35
ATOM	1188	N	ASP	313	66.633	30.060	5.855	1.00	22.16
ATOM	1189	CA	ASP	313	65.430	30.589	6.494	1.00	21.37
ATOM	1190	CB	ASP	313	64.625	31.431	5.499	1.00	25.11
ATOM	1191	CG	ASP	313	65.380	32.666	5.025	1.00	31.54
ATOM	1192	OD1	ASP	313	65.119	33.115	3.890	1.00	35.35
ATOM	1193	OD2	ASP	313	66.225	33.193	5.783	1.00	35.37
ATOM	1194	C	ASP	313	64.524	29.535	7.120	1.00	21.11
ATOM	1195	O	ASP	313	63.904	29.783	8.158	1.00	23.68
ATOM	1196	N	THR	314	64.440	28.367	6.489	1.00	22.88
ATOM	1197	CA	THR	314	63.591	27.281	6.981	1.00	22.81
ATOM	1198	CB	THR	314	63.472	26.155	5.927	1.00	26.00
ATOM	1199	OG1	THR	314	62.873	26.679	4.732	1.00	20.14
ATOM	1200	CG2	THR	314	62.629	25.010	6.457	1.00	17.51
ATOM	1201	C	THR	314	64.086	26.706	8.310	1.00	19.46
ATOM	1202	O	THR	314	63.312	26.529	9.247	1.00	19.33
ATOM	1203	N	GLU	315	65.381	26.431	8.392	1.00	17.49
ATOM	1204	CA	GLU	315	65.965	25.885	9.611	1.00	20.62
ATOM	1205	CB	GLU	315	67.426	25.514	9.358	1.00	14.39
ATOM	1206	CG	GLU	315	67.539	24.339	8.400	1.00	13.07
ATOM	1207	CD	GLU	315	68.923	24.125	7.835	1.00	14.98
ATOM	1208	OE1	GLU	315	69.634	25.116	7.552	1.00	17.71
ATOM	1209	OE2	GLU	315	69.287	22.948	7.651	1.00	17.88
ATOM	1210	C	GLU	315	65.810	26.883	10.762	1.00	20.57
ATOM	1211	O	GLU	315	65.368	26.518	11.854	1.00	18.43
ATOM	1212	N	VAL	316	66.096	28.154	10.488	1.00	19.19
ATOM	1213	CA	VAL	316	65.955	29.203	11.490	1.00	16.53
ATOM	1214	CB	VAL	316	66.418	30.567	10.933	1.00	17.42
ATOM	1215	CG1	VAL	316	66.149	31.687	11.940	1.00	13.89
ATOM	1216	CG2	VAL	316	67.900	30.506	10.594	1.00	14.31
ATOM	1217	C	VAL	316	64.488	29.291	11.927	1.00	19.53
ATOM	1218	O	VAL	316	64.191	29.448	13.110	1.00	19.86
ATOM	1219	N	ALA	317	63.575	29.159	10.970	1.00	19.02
ATOM	1220	CA	ALA	317	62.145	29.215	11.254	1.00	16.95
ATOM	1221	CB	ALA	317	61.357	29.239	9.951	1.00	17.68
ATOM	1222	C	ALA	317	61.674	28.047	12.126	1.00	14.13
ATOM	1223	O	ALA	317	60.875	28.228	13.045	1.00	15.34
ATOM	1224	N	LEU	318	62.154	26.847	11.819	1.00	17.41
ATOM	1225	CA	LEU						

ATOM	1227	CG	LEU	318	61.443	24.209	10.473	1.00	19.02
ATOM	1228	CD1	LEU	318	62.105	23.128	9.646	1.00	16.10
ATOM	1229	CD2	LEU	318	59.987	23.875	10.735	1.00	11.32
ATOM	1230	C	LEU	318	62.399	25.685	13.954	1.00	22.38
ATOM	1231	O	LEU	318	61.782	25.278	14.945	1.00	21.64
ATOM	1232	N	LEU	319	63.619	26.207	14.016	1.00	20.97
ATOM	1233	CA	LEU	319	64.338	26.344	15.270	1.00	19.71
ATOM	1234	CB	LEU	319	65.715	26.951	15.005	1.00	20.56
ATOM	1235	CG	LEU	319	66.722	27.036	16.152	1.00	32.05
ATOM	1236	CD1	LEU	319	66.704	25.760	16.963	1.00	33.15
ATOM	1237	CD2	LEU	319	68.109	27.303	15.590	1.00	28.25
ATOM	1238	C	LEU	319	63.496	27.254	16.164	1.00	20.66
ATOM	1239	O	LEU	319	63.215	26.920	17.313	1.00	24.47
ATOM	1240	N	GLN	320	63.026	28.365	15.604	1.00	19.25
ATOM	1241	CA	GLN	320	62.191	29.307	16.346	1.00	19.02
ATOM	1242	CB	GLN	320	61.842	30.526	15.488	1.00	19.11
ATOM	1243	CG	GLN	320	63.032	31.377	15.101	1.00	20.02
ATOM	1244	CD	GLN	320	62.665	32.562	14.224	1.00	23.65
ATOM	1245	OE1	GLN	320	63.487	33.445	13.997	1.00	22.68
ATOM	1246	NE2	GLN	320	61.440	32.574	13.704	1.00	20.77
ATOM	1247	C	GLN	320	60.905	28.635	16.811	1.00	20.52
ATOM	1248	O	GLN	320	60.465	28.845	17.938	1.00	22.04
ATOM	1249	N	ALA	321	60.306	27.825	15.942	1.00	21.01
ATOM	1250	CA	ALA	321	59.069	27.128	16.280	1.00	16.83
ATOM	1251	CB	ALA	321	58.556	26.358	15.079	1.00	16.58
ATOM	1252	C	ALA	321	59.288	26.185	17.462	1.00	18.15
ATOM	1253	O	ALA	321	58.427	26.069	18.344	1.00	13.03
ATOM	1254	N	VAL	322	60.442	25.523	17.481	1.00	14.89
ATOM	1255	CA	VAL	322	60.774	24.599	18.559	1.00	19.05
ATOM	1256	CB	VAL	322	62.051	23.779	18.233	1.00	21.50
ATOM	1257	CG1	VAL	322	62.510	22.990	19.457	1.00	21.49
ATOM	1258	CG2	VAL	322	61.773	22.819	17.073	1.00	15.42
ATOM	1259	C	VAL	322	60.947	25.375	19.867	1.00	19.89
ATOM	1260	O	VAL	322	60.478	24.940	20.919	1.00	21.58
ATOM	1261	N	LEU	323	61.591	26.537	19.788	1.00	20.25
ATOM	1262	CA	LEU	323	61.804	27.387	20.959	1.00	19.32
ATOM	1263	CB	LEU	323	62.683	28.586	20.597	1.00	12.95
ATOM	1264	CG	LEU	323	64.129	28.273	20.217	1.00	20.70
ATOM	1265	CD1	LEU	323	64.805	29.503	19.641	1.00	13.23
ATOM	1266	CD2	LEU	323	64.883	27.767	21.438	1.00	22.91
ATOM	1267	C	LEU	323	60.468	27.884	21.497	1.00	20.25
ATOM	1268	O	LEU	323	60.251	27.918	22.706	1.00	25.88
ATOM	1269	N	LEU	324	59.571	28.251	20.587	1.00	23.08
ATOM	1270	CA	LEU	324	58.248	28.753	20.944	1.00	21.24
ATOM	1271	CB	LEU	324	57.555	29.333	19.70		



ATOM	1274	CD2	LEU	324	55.545	30.162	18.498	1.00	17.90
ATOM	1275	C	LEU	324	57.342	27.706	21.598	1.00	21.54
ATOM	1276	O	LEU	324	56.742	27.967	22.642	1.00	23.41
ATOM	1277	N	MET	325	57.249	26.521	21.003	1.00	24.63
ATOM	1278	CA	MET	325	56.380	25.476	21.545	1.00	25.35
ATOM	1279	CB	MET	325	55.901	24.536	20.430	1.00	25.53
ATOM	1280	CG	MET	325	55.235	25.220	19.232	1.00	21.89
ATOM	1281	SD	MET	325	53.871	26.337	19.649	1.00	25.50
ATOM	1282	CE	MET	325	52.705	25.250	20.397	1.00	17.66
ATOM	1283	C	MET	325	57.031	24.676	22.675	1.00	27.58
ATOM	1284	O	MET	325	56.988	23.450	22.690	1.00	28.61
ATOM	1285	N	SER	326	57.613	25.376	23.638	1.00	27.98
ATOM	1286	CA	SER	326	58.265	24.718	24.757	1.00	31.60
ATOM	1287	CB	SER	326	59.527	25.493	25.155	1.00	35.80
ATOM	1288	OG	SER	326	60.123	24.966	26.327	1.00	43.74
ATOM	1289	C	SER	326	57.313	24.624	25.939	1.00	32.12
ATOM	1290	O	SER	326	56.590	25.574	26.240	1.00	30.91
ATOM	1291	N	THR	327	57.276	23.464	26.583	1.00	35.41
ATOM	1292	CA	THR	327	56.420	23.278	27.747	1.00	39.61
ATOM	1293	CB	THR	327	55.777	21.890	27.758	1.00	38.84
ATOM	1294	OG1	THR	327	56.784	20.890	27.538	1.00	42.53
ATOM	1295	CG2	THR	327	54.716	21.802	26.679	1.00	40.78
ATOM	1296	C	THR	327	57.232	23.471	29.022	1.00	43.86
ATOM	1297	O	THR	327	56.785	23.133	30.118	1.00	42.40
ATOM	1298	N	ASP	328	58.417	24.054	28.869	1.00	47.35
ATOM	1299	CA	ASP	328	59.309	24.308	29.987	1.00	49.43
ATOM	1300	CB	ASP	328	60.750	24.358	29.482	1.00	58.03
ATOM	1301	CG	ASP	328	61.718	23.687	30.425	1.00	72.16
ATOM	1302	OD1	ASP	328	61.816	24.117	31.595	1.00	82.32
ATOM	1303	OD2	ASP	328	62.378	22.720	29.994	1.00	81.63
ATOM	1304	C	ASP	328	58.951	25.625	30.676	1.00	47.99
ATOM	1305	O	ASP	328	59.830	26.373	31.093	1.00	53.33
ATOM	1306	N	ARG	329	57.657	25.910	30.780	1.00	48.33
ATOM	1307	CA	ARG	329	57.177	27.135	31.413	1.00	47.67
ATOM	1308	CB	ARG	329	56.562	28.091	30.379	1.00	47.64
ATOM	1309	CG	ARG	329	57.550	28.802	29.450	1.00	47.87
ATOM	1310	CD	ARG	329	57.893	27.968	28.226	1.00	44.00
ATOM	1311	NE	ARG	329	58.759	28.682	27.288	1.00	41.17
ATOM	1312	CZ	ARG	329	60.087	28.605	27.283	1.00	48.58
ATOM	1313	NH1	ARG	329	60.719	27.848	28.172	1.00	52.94
ATOM	1314	NH2	ARG	329	60.784	29.257	26.362	1.00	43.16
ATOM	1315	C	ARG	329	56.126	26.778	32.457	1.00	48.01
ATOM	1316	O	ARG	329	55.573	25.677	32.437	1.00	50.22
ATOM	1317	N	SER	330	55.832	27.716	33.351	1.00	47.37
ATOM	1318	CA	SER	330	54.848	27.490	34.402	1.00	47.64
ATOM									



ATOM	1321	O	SER	330	53.460	29.252	33.548	1.00	48.49
ATOM	1322	N	GLY	331	52.421	27.424	34.359	1.00	44.16
ATOM	1323	CA	GLY	331	51.090	27.956	34.123	1.00	41.44
ATOM	1324	C	GLY	331	50.424	27.660	32.790	1.00	42.83
ATOM	1325	O	GLY	331	49.478	28.351	32.413	1.00	45.88
ATOM	1326	N	LEU	332	50.889	26.643	32.075	1.00	40.10
ATOM	1327	CA	LEU	332	50.288	26.300	30.789	1.00	39.27
ATOM	1328	CB	LEU	332	51.301	25.596	29.885	1.00	37.42
ATOM	1329	CG	LEU	332	52.436	26.426	29.291	1.00	35.35
ATOM	1330	CD1	LEU	332	53.374	25.505	28.530	1.00	31.61
ATOM	1331	CD2	LEU	332	51.875	27.511	28.376	1.00	31.82
ATOM	1332	C	LEU	332	49.058	25.415	30.951	1.00	39.32
ATOM	1333	O	LEU	332	49.060	24.467	31.738	1.00	42.74
ATOM	1334	N	LEU	333	48.009	25.730	30.202	1.00	37.62
ATOM	1335	CA	LEU	333	46.778	24.953	30.241	1.00	41.30
ATOM	1336	CB	LEU	333	45.586	25.835	29.852	1.00	43.52
ATOM	1337	CG	LEU	333	45.125	26.904	30.848	1.00	49.39
ATOM	1338	CD1	LEU	333	44.296	27.970	30.142	1.00	46.19
ATOM	1339	CD2	LEU	333	44.330	26.248	31.968	1.00	51.29
ATOM	1340	C	LEU	333	46.859	23.762	29.285	1.00	41.39
ATOM	1341	O	LEU	333	46.565	22.628	29.657	1.00	43.41
ATOM	1342	N	CYA	334	47.317	24.024	28.067	1.00	42.18
ATOM	1343	CA	CYA	334	47.409	23.003	27.029	1.00	39.56
ATOM	1344	CB	CYA	334	47.004	23.616	25.691	1.00	45.48
ATOM	1345	SG	CYA	334	45.517	24.616	25.785	1.00	51.57
ATOM	1346	AS	CYA	334	44.187	22.808	25.555	1.00	90.90
ATOM	1347	C	CYA	334	48.776	22.347	26.891	1.00	38.28
ATOM	1348	O	CYA	334	49.273	22.178	25.778	1.00	40.95
ATOM	1349	N	VAL	335	49.345	21.913	28.009	1.00	36.05
ATOM	1350	CA	VAL	335	50.661	21.278	28.006	1.00	35.78
ATOM	1351	CB	VAL	335	50.996	20.679	29.399	1.00	35.53
ATOM	1352	CG1	VAL	335	52.413	20.123	29.407	1.00	32.76
ATOM	1353	CG2	VAL	335	50.822	21.729	30.490	1.00	28.87
ATOM	1354	C	VAL	335	50.776	20.170	26.950	1.00	36.41
ATOM	1355	O	VAL	335	51.756	20.104	26.202	1.00	34.26
ATOM	1356	N	ASP	336	49.756	19.323	26.880	1.00	38.42
ATOM	1357	CA	ASP	336	49.736	18.209	25.942	1.00	39.71
ATOM	1358	CB	ASP	336	48.485	17.359	26.179	1.00	51.53
ATOM	1359	CG	ASP	336	48.534	16.028	25.452	1.00	65.98
ATOM	1360	OD1	ASP	336	49.240	15.114	25.934	1.00	70.75
ATOM	1361	OD2	ASP	336	47.858	15.891	24.406	1.00	72.15
ATOM	1362	C	ASP	336	49.794	18.668	24.486	1.00	37.72
ATOM	1363	O	ASP	336	50.686	18.259	23.733	1.00	32.08
ATOM	1364	N	LYS	337	48.858	19.532	24.100	1.00	33.78
ATOM	1365	CA	LYS	337	48.797	20.040	22.731	1.00	

ATOM	1368	O	LYS	337	50.607	20.512	21.220	1.00	28.41
ATOM	1369	N	ILE	338	50.705	21.449	23.267	1.00	27.56
ATOM	1370	CA	ILE	338	51.964	22.138	23.022	1.00	25.03
ATOM	1371	CB	ILE	338	52.274	23.149	24.144	1.00	19.49
ATOM	1372	CG2	ILE	338	53.577	23.876	23.859	1.00	19.00
ATOM	1373	CG1	ILE	338	51.135	24.167	24.232	1.00	21.97
ATOM	1374	CD1	ILE	338	51.277	25.175	25.348	1.00	26.67
ATOM	1375	C	ILE	338	53.119	21.153	22.826	1.00	29.97
ATOM	1376	O	ILE	338	53.935	21.328	21.914	1.00	31.00
ATOM	1377	N	GLU	339	53.165	20.100	23.642	1.00	33.52
ATOM	1378	CA	GLU	339	54.213	19.080	23.516	1.00	35.34
ATOM	1379	CB	GLU	339	54.136	18.062	24.659	1.00	39.97
ATOM	1380	CG	GLU	339	54.653	18.585	25.986	1.00	53.23
ATOM	1381	CD	GLU	339	54.549	17.579	27.126	1.00	61.16
ATOM	1382	OE1	GLU	339	53.602	16.759	27.131	1.00	64.30
ATOM	1383	OE2	GLU	339	55.412	17.622	28.031	1.00	57.76
ATOM	1384	C	GLU	339	54.091	18.353	22.178	1.00	31.63
ATOM	1385	O	GLU	339	55.086	18.123	21.491	1.00	28.96
ATOM	1386	N	LYS	340	52.861	18.006	21.810	1.00	30.95
ATOM	1387	CA	LYS	340	52.602	17.313	20.554	1.00	31.58
ATOM	1388	CB	LYS	340	51.121	16.966	20.438	1.00	31.83
ATOM	1389	C	LYS	340	53.057	18.159	19.358	1.00	29.84
ATOM	1390	O	LYS	340	53.696	17.640	18.438	1.00	31.58
ATOM	1391	N	SER	341	52.765	19.460	19.388	1.00	25.33
ATOM	1392	CA	SER	341	53.165	20.351	18.297	1.00	23.92
ATOM	1393	CB	SER	341	52.468	21.707	18.400	1.00	24.02
ATOM	1394	OG	SER	341	52.700	22.302	19.657	1.00	48.88
ATOM	1395	C	SER	341	54.677	20.533	18.240	1.00	24.39
ATOM	1396	O	SER	341	55.254	20.593	17.150	1.00	24.71
ATOM	1397	N	GLN	342	55.324	20.606	19.405	1.00	25.45
ATOM	1398	CA	GLN	342	56.777	20.751	19.437	1.00	26.66
ATOM	1399	CB	GLN	342	57.311	20.975	20.853	1.00	22.77
ATOM	1400	CG	GLN	342	58.805	21.307	20.840	1.00	25.76
ATOM	1401	CD	GLN	342	59.427	21.371	22.214	1.00	28.46
ATOM	1402	OE1	GLN	342	59.342	20.422	22.990	1.00	34.22
ATOM	1403	NE2	GLN	342	60.080	22.483	22.517	1.00	30.01
ATOM	1404	C	GLN	342	57.425	19.504	18.843	1.00	23.37
ATOM	1405	O	GLN	342	58.414	19.598	18.106	1.00	23.65
ATOM	1406	N	GLU	343	56.864	18.340	19.162	1.00	21.48
ATOM	1407	CA	GLU	343	57.370	17.076	18.641	1.00	20.74
ATOM	1408	CB	GLU	343	56.599	15.902	19.247	1.00	22.09
ATOM	1409	C	GLU	343	57.225	17.094	17.119	1.00	19.18
ATOM	1410	O	GLU	343	58.156	16.743	16.393	1.00	21.11
ATOM	1411	N	ALA	344	56.077	17.570	16.648	1.00	19.93
ATOM	1412	CA	ALA	344	55.803	17.662	15.217	1.	

ATOM	1415	O	ALA	344	57.432	18.140	13.514	1.00	25.13
ATOM	1416	N	TYR	345	57.105	19.722	15.088	1.00	21.31
ATOM	1417	CA	TYR	345	58.107	20.631	14.531	1.00	15.93
ATOM	1418	CB	TYR	345	58.127	21.969	15.282	1.00	17.29
ATOM	1419	CG	TYR	345	57.049	22.927	14.833	1.00	16.11
ATOM	1420	CD1	TYR	345	56.017	23.296	15.689	1.00	9.93
ATOM	1421	CE1	TYR	345	54.999	24.138	15.263	1.00	16.95
ATOM	1422	CD2	TYR	345	57.041	23.431	13.531	1.00	19.84
ATOM	1423	CE2	TYR	345	56.026	24.276	13.094	1.00	17.13
ATOM	1424	CZ	TYR	345	55.005	24.622	13.963	1.00	18.12
ATOM	1425	OH	TYR	345	53.980	25.430	13.530	1.00	26.25
ATOM	1426	C	TYR	345	59.493	20.008	14.554	1.00	20.65
ATOM	1427	O	TYR	345	60.240	20.129	13.583	1.00	20.75
ATOM	1428	N	LEU	346	59.832	19.337	15.655	1.00	22.14
ATOM	1429	CA	LEU	346	61.134	18.684	15.803	1.00	19.43
ATOM	1430	CB	LEU	346	61.267	18.041	17.186	1.00	19.92
ATOM	1431	CG	LEU	346	61.683	18.945	18.347	1.00	25.56
ATOM	1432	CD1	LEU	346	61.440	18.244	19.677	1.00	22.06
ATOM	1433	CD2	LEU	346	63.147	19.332	18.197	1.00	17.62
ATOM	1434	C	LEU	346	61.359	17.635	14.723	1.00	19.30
ATOM	1435	O	LEU	346	62.441	17.560	14.142	1.00	22.84
ATOM	1436	N	LEU	347	60.337	16.826	14.456	1.00	25.17
ATOM	1437	CA	LEU	347	60.423	15.790	13.427	1.00	24.55
ATOM	1438	CB	LEU	347	59.187	14.892	13.453	1.00	25.47
ATOM	1439	CG	LEU	347	59.256	13.654	14.345	1.00	30.65
ATOM	1440	CD1	LEU	347	57.941	12.890	14.258	1.00	34.28
ATOM	1441	CD2	LEU	347	60.416	12.765	13.908	1.00	28.26
ATOM	1442	C	LEU	347	60.584	16.400	12.042	1.00	24.00
ATOM	1443	O	LEU	347	61.399	15.932	11.245	1.00	29.74
ATOM	1444	N	ALA	348	59.809	17.443	11.761	1.00	22.72
ATOM	1445	CA	ALA	348	59.875	18.125	10.475	1.00	19.19
ATOM	1446	CB	ALA	348	58.789	19.188	10.388	1.00	22.73
ATOM	1447	C	ALA	348	61.246	18.762	10.316	1.00	20.34
ATOM	1448	O	ALA	348	61.881	18.633	9.274	1.00	23.94
ATOM	1449	N	PHE	349	61.707	19.402	11.388	1.00	22.19
ATOM	1450	CA	PHE	349	63.001	20.078	11.435	1.00	19.41
ATOM	1451	CB	PHE	349	63.185	20.701	12.832	1.00	17.45
ATOM	1452	CG	PHE	349	64.371	21.632	12.963	1.00	18.70
ATOM	1453	CD1	PHE	349	65.183	21.943	11.874	1.00	19.09
ATOM	1454	CD2	PHE	349	64.669	22.203	14.199	1.00	21.81
ATOM	1455	CE1	PHE	349	66.270	22.811	12.012	1.00	21.49
ATOM	1456	CE2	PHE	349	65.753	23.072	14.351	1.00	18.58
ATOM	1457	CZ	PHE	349	66.555	23.376	13.256	1.00	18.67
ATOM	1458	C	PHE	349	64.110	19.071	11.136	1.00	20.96
ATOM	1459	O	PHE	349	64.967	19.311	10.283</		

ATOM	1462	CB	GLU	350	64.794	15.721	12.591	1.00	28.90
ATOM	1463	CG	GLU	350	65.738	14.542	12.413	1.00	39.36
ATOM	1464	CD	GLU	350	65.603	13.497	13.505	1.00	41.62
ATOM	1465	OE1	GLU	350	64.475	13.260	13.988	1.00	43.67
ATOM	1466	OE2	GLU	350	66.636	12.908	13.876	1.00	49.64
ATOM	1467	C-	GLU	350	65.100	16.385	10.203	1.00	27.12
ATOM	1468	O	GLU	350	66.158	16.288	9.577	1.00	27.44
ATOM	1469	N	HIS	351	63.918	16.088	9.678	1.00	27.36
ATOM	1470	CA	HIS	351	63.787	15.591	8.318	1.00	23.97
ATOM	1471	CB	HIS	351	62.366	15.087	8.090	1.00	22.89
ATOM	1472	CG	HIS	351	61.991	13.945	8.986	1.00	24.58
ATOM	1473	CD2	HIS	351	62.736	13.209	9.846	1.00	25.83
ATOM	1474	ND1	HIS	351	60.709	13.448	9.073	1.00	26.50
ATOM	1475	CE1	HIS	351	60.677	12.460	9.948	1.00	24.81
ATOM	1476	NE2	HIS	351	61.896	12.295	10.431	1.00	28.42
ATOM	1477	C	HIS	351	64.200	16.635	7.278	1.00	24.22
ATOM	1478	O	HIS	351	64.757	16.287	6.236	1.00	25.79
ATOM	1479	N	TYR	352	63.969	17.912	7.572	1.00	21.04
ATOM	1480	CA	TYR	352	64.363	18.974	6.654	1.00	18.98
ATOM	1481	CB	TYR	352	63.770	20.321	7.067	1.00	17.08
ATOM	1482	CG	TYR	352	64.127	21.413	6.090	1.00	21.83
ATOM	1483	CD1	TYR	352	63.537	21.467	4.828	1.00	20.07
ATOM	1484	CE1	TYR	352	63.941	22.411	3.883	1.00	23.51
ATOM	1485	CD2	TYR	352	65.121	22.339	6.388	1.00	19.94
ATOM	1486	CE2	TYR	352	65.531	23.284	5.452	1.00	20.85
ATOM	1487	CZ	TYR	352	64.942	23.313	4.203	1.00	24.80
ATOM	1488	OH	TYR	352	65.380	24.221	3.269	1.00	26.74
ATOM	1489	C	TYR	352	65.889	19.055	6.624	1.00	20.58
ATOM	1490	O	TYR	352	66.492	19.276	5.570	1.00	22.72
ATOM	1491	N	VAL	353	66.508	18.877	7.789	1.00	28.34
ATOM	1492	CA	VAL	353	67.967	18.892	7.904	1.00	22.38
ATOM	1493	CB	VAL	353	68.419	18.755	9.389	1.00	26.46
ATOM	1494	CG1	VAL	353	69.915	18.527	9.478	1.00	20.92
ATOM	1495	CG2	VAL	353	68.053	20.009	10.165	1.00	22.46
ATOM	1496	C	VAL	353	68.518	17.725	7.078	1.00	23.51
ATOM	1497	O	VAL	353	69.535	17.865	6.391	1.00	24.73
ATOM	1498	N	ASN	354	67.850	16.575	7.158	1.00	20.93
ATOM	1499	CA	ASN	354	68.252	15.392	6.397	1.00	27.25
ATOM	1500	CB	ASN	354	67.320	14.210	6.680	1.00	28.43
ATOM	1501	CG	ASN	354	67.521	13.607	8.058	1.00	31.50
ATOM	1502	OD1	ASN	354	68.565	13.787	8.692	1.00	37.79
ATOM	1503	ND2	ASN	354	66.521	12.867	8.524	1.00	26.44
ATOM	1504	C	ASN	354	68.182	15.721	4.908	1.00	31.27
ATOM	1505	O	ASN	354	69.066	15.347	4.134	1.00	34.22
ATOM	1506	N	HIS	355	67.124	16.429	4.520	1.00	30.49
ATOM	1507								



ATOM	1509	CG	HIS	355	65.319	18.103	1.625	1.00	37.76
ATOM	1510	CD2	HIS	355	65.439	19.382	1.196	1.00	35.28
ATOM	1511	ND1	HIS	355	64.913	17.369	0.532	1.00	34.93
ATOM	1512	CE1	HIS	355	64.789	18.169	-0.513	1.00	34.84
ATOM	1513	NE2	HIS	355	65.104	19.394	-0.135	1.00	33.13
ATOM	1514	C-	HIS	355	68.016	17.748	2.610	1.00	24.66
ATOM	1515	O	HIS	355	68.420	17.630	1.456	1.00	26.62
ATOM	1516	N	ARG	356	68.487	18.670	3.448	1.00	25.86
ATOM	1517	CA	ARG	356	69.536	19.608	3.040	1.00	26.94
ATOM	1518	CB	ARG	356	69.620	20.791	3.996	1.00	20.57
ATOM	1519	CG	ARG	356	68.453	21.727	3.899	1.00	19.69
ATOM	1520	CD	ARG	356	68.866	23.110	4.340	1.00	23.81
ATOM	1521	NE	ARG	356	69.768	23.746	3.388	1.00	23.14
ATOM	1522	CZ	ARG	356	70.641	24.697	3.702	1.00	24.11
ATOM	1523	NH1	ARG	356	70.755	25.129	4.949	1.00	26.29
ATOM	1524	NH2	ARG	356	71.384	25.242	2.754	1.00	32.79
ATOM	1525	C	ARG	356	70.921	19.002	2.875	1.00	29.38
ATOM	1526	O	ARG	356	71.795	19.607	2.257	1.00	32.91
ATOM	1527	N	LYS	357	71.133	17.848	3.498	1.00	33.39
ATOM	1528	CA	LYS	357	72.401	17.128	3.417	1.00	35.97
ATOM	1529	CB	LYS	357	72.479	16.363	2.089	1.00	40.55
ATOM	1530	CG	LYS	357	71.327	15.381	1.891	1.00	44.03
ATOM	1531	CD	LYS	357	71.360	14.722	0.523	1.00	52.31
ATOM	1532	CE	LYS	357	70.171	13.787	0.343	1.00	56.99
ATOM	1533	NZ	LYS	357	70.208	13.085	-0.970	1.00	64.78
ATOM	1534	C	LYS	357	73.657	17.981	3.629	1.00	38.55
ATOM	1535	O	LYS	357	74.518	18.079	2.748	1.00	42.50
ATOM	1536	N	HIS	358	73.751	18.601	4.802	1.00	35.00
ATOM	1537	CA	HIS	358	74.906	19.418	5.155	1.00	32.94
ATOM	1538	CB	HIS	358	74.732	20.018	6.552	1.00	27.62
ATOM	1539	CG	HIS	358	73.669	21.067	6.643	1.00	26.64
ATOM	1540	CD2	HIS	358	72.330	20.968	6.819	1.00	20.85
ATOM	1541	ND1	HIS	358	73.950	22.416	6.587	1.00	24.71
ATOM	1542	CE1	HIS	358	72.831	23.103	6.724	1.00	21.02
ATOM	1543	NE2	HIS	358	71.834	22.248	6.865	1.00	21.42
ATOM	1544	C	HIS	358	76.140	18.520	5.176	1.00	36.60
ATOM	1545	O	HIS	358	76.072	17.379	5.635	1.00	38.73
ATOM	1546	N	ASN	359	77.267	19.037	4.702	1.00	41.40
ATOM	1547	CA	ASN	359	78.515	18.277	4.689	1.00	45.02
ATOM	1548	CB	ASN	359	79.441	18.799	3.587	1.00	42.57
ATOM	1549	C	ASN	359	79.193	18.386	6.058	1.00	46.59
ATOM	1550	O	ASN	359	80.405	18.588	6.150	1.00	52.31
ATOM	1551	N	ILE	360	78.400	18.254	7.117	1.00	45.14
ATOM	1552	CA	ILE	360	78.896	18.348	8.487	1.00	43.69
ATOM	1553	CB	ILE	360	78.330	19.597	9.207	1.00	40.08
ATOM	1554	CG2	ILE	360					



ATOM	1556	CD1	ILE	360	78.057	22.115	8.954	1.00	44.93
ATOM	1557	C	ILE	360	78.452	17.101	9.242	1.00	43.63
ATOM	1558	O	ILE	360	77.257	16.797	9.313	1.00	45.20
ATOM	1559	N	PRO	361	79.413	16.337	9.780	1.00	43.91
ATOM	1560	CD	PRO	361	80.871	16.540	9.699	1.00	47.07
ATOM	1561	CA	PRO	361	79.087	15.118	10.526	1.00	41.66
ATOM	1562	CB	PRO	361	80.462	14.495	10.782	1.00	43.73
ATOM	1563	CG	PRO	361	81.383	15.679	10.830	1.00	45.45
ATOM	1564	C	PRO	361	78.332	15.403	11.832	1.00	36.42
ATOM	1565	O	PRO	361	78.679	16.325	12.572	1.00	35.74
ATOM	1566	N	HIS	362	77.291	14.610	12.088	1.00	33.14
ATOM	1567	CA	HIS	362	76.462	14.726	13.292	1.00	34.09
ATOM	1568	CB	HIS	362	77.288	14.413	14.547	1.00	33.82
ATOM	1569	CG	HIS	362	78.132	13.181	14.424	1.00	36.04
ATOM	1570	CD2	HIS	362	77.793	11.885	14.224	1.00	34.77
ATOM	1571	ND1	HIS	362	79.509	13.212	14.482	1.00	37.16
ATOM	1572	CE1	HIS	362	79.983	11.990	14.325	1.00	37.16
ATOM	1573	NE2	HIS	362	78.962	11.165	14.167	1.00	40.13
ATOM	1574	C	HIS	362	75.829	16.110	13.417	1.00	31.00
ATOM	1575	O	HIS	362	75.617	16.608	14.525	1.00	30.22
ATOM	1576	N	PHE	363	75.478	16.690	12.272	1.00	33.06
ATOM	1577	CA	PHE	363	74.878	18.021	12.200	1.00	28.08
ATOM	1578	CB	PHE	363	74.503	18.355	10.747	1.00	25.26
ATOM	1579	CG	PHE	363	73.923	19.733	10.567	1.00	24.91
ATOM	1580	CD1	PHE	363	74.750	20.817	10.320	1.00	27.60
ATOM	1581	CD2	PHE	363	72.552	19.948	10.664	1.00	25.52
ATOM	1582	CE1	PHE	363	74.221	22.100	10.175	1.00	29.70
ATOM	1583	CE2	PHE	363	72.014	21.227	10.522	1.00	25.88
ATOM	1584	CZ	PHE	363	72.850	22.304	10.278	1.00	21.49
ATOM	1585	C	PHE	363	73.659	18.201	13.099	1.00	23.79
ATOM	1586	O	PHE	363	73.587	19.164	13.863	1.00	24.48
ATOM	1587	N	TRP	364	72.707	17.277	13.012	1.00	23.13
ATOM	1588	CA	TRP	364	71.484	17.369	13.805	1.00	25.06
ATOM	1589	CB	TRP	364	70.536	16.201	13.494	1.00	21.17
ATOM	1590	CG	TRP	364	69.247	16.220	14.271	1.00	23.14
ATOM	1591	CD2	TRP	364	68.261	17.266	14.296	1.00	27.68
ATOM	1592	CE2	TRP	364	67.229	16.845	15.165	1.00	28.31
ATOM	1593	CE3	TRP	364	68.149	18.517	13.671	1.00	26.46
ATOM	1594	CD1	TRP	364	68.784	15.241	15.096	1.00	23.76
ATOM	1595	NE1	TRP	364	67.576	15.607	15.637	1.00	32.12
ATOM	1596	CZ2	TRP	364	66.100	17.628	15.427	1.00	25.63
ATOM	1597	CZ3	TRP	364	67.028	19.294	13.931	1.00	25.55
ATOM	1598	CH2	TRP	364	66.017	18.845	14.803	1.00	29.79
ATOM	1599	C	TRP	364	71.715	17.531	15.312	1.00	27.80
ATOM	1600	O	TRP	364	71.212	18.486	15.904	1.00	

ATOM	1603	CA	PRO	365	72.687	16.757	17.397	1.00	27.97
ATOM	1604	CB	PRO	365	73.506	15.512	17.752	1.00	26.50
ATOM	1605	CG	PRO	365	73.057	14.509	16.757	1.00	33.47
ATOM	1606	C	PRO	365	73.457	18.043	17.709	1.00	27.10
ATOM	1607	O	PRO	365	73.154	18.736	18.681	1.00	26.88
ATOM	1608	N	LYS	366	74.440	18.365	16.873	1.00	26.99
ATOM	1609	CA	LYS	366	75.230	19.577	17.061	1.00	30.69
ATOM	1610	CB	LYS	366	76.275	19.708	15.957	1.00	28.53
ATOM	1611	CG	LYS	366	77.481	18.804	16.106	1.00	28.89
ATOM	1612	CD	LYS	366	78.430	19.027	14.939	1.00	32.51
ATOM	1613	CE	LYS	366	79.743	18.294	15.116	1.00	38.52
ATOM	1614	NZ	LYS	366	80.632	18.506	13.939	1.00	45.28
ATOM	1615	C	LYS	366	74.349	20.831	17.079	1.00	36.18
ATOM	1616	O	LYS	366	74.472	21.672	17.972	1.00	39.82
ATOM	1617	N	LEU	367	73.464	20.950	16.091	1.00	37.54
ATOM	1618	CA	LEU	367	72.557	22.092	15.994	1.00	36.14
ATOM	1619	CB	LEU	367	71.803	22.070	14.659	1.00	32.20
ATOM	1620	CG	LEU	367	70.764	23.179	14.447	1.00	36.16
ATOM	1621	CD1	LEU	367	71.402	24.567	14.618	1.00	20.60
ATOM	1622	CD2	LEU	367	70.139	23.030	13.065	1.00	34.30
ATOM	1623	C	LEU	367	71.561	22.060	17.143	1.00	36.84
ATOM	1624	O	LEU	367	71.231	23.091	17.729	1.00	36.94
ATOM	1625	N	LEU	368	71.083	20.866	17.459	1.00	37.81
ATOM	1626	CA	LEU	368	70.130	20.683	18.536	1.00	34.83
ATOM	1627	CB	LEU	368	69.763	19.205	18.622	1.00	36.98
ATOM	1628	CG	LEU	368	68.421	18.777	19.205	1.00	40.34
ATOM	1629	CD1	LEU	368	67.276	19.595	18.619	1.00	36.28
ATOM	1630	CD2	LEU	368	68.241	17.299	18.908	1.00	39.39
ATOM	1631	C	LEU	368	70.755	21.182	19.843	1.00	38.32
ATOM	1632	O	LEU	368	70.059	21.711	20.707	1.00	41.87
ATOM	1633	N	MET	369	72.075	21.057	19.962	1.00	39.46
ATOM	1634	CA	MET	369	72.790	21.515	21.154	1.00	40.12
ATOM	1635	CB	MET	369	74.219	20.971	21.168	1.00	41.26
ATOM	1636	CG	MET	369	74.307	19.493	21.521	1.00	47.83
ATOM	1637	SD	MET	369	75.961	18.810	21.289	1.00	55.72
ATOM	1638	CE	MET	369	76.809	19.474	22.727	1.00	54.37
ATOM	1639	C	MET	369	72.805	23.039	21.251	1.00	42.81
ATOM	1640	O	MET	369	72.990	23.601	22.335	1.00	47.81
ATOM	1641	N	LYS	370	72.622	23.708	20.115	1.00	40.09
ATOM	1642	CA	LYS	370	72.588	25.165	20.080	1.00	33.65
ATOM	1643	CB	LYS	370	72.751	25.677	18.650	1.00	30.83
ATOM	1644	CG	LYS	370	74.138	25.435	18.078	1.00	30.98
ATOM	1645	CD	LYS	370	75.188	26.198	18.867	1.00	37.82
ATOM	1646	CE	LYS	370	76.591	25.938	18.351	1.00	36.05
ATOM	1647	NZ	LYS	370	77.034	24.562	18.667		

ATOM	1650	N	VAL	371	70.277	24.826	20.779	1.00	31.90
ATOM	1651	CA	VAL	371	69.006	25.197	21.395	1.00	31.77
ATOM	1652	CB	VAL	371	67.933	24.092	21.214	1.00	30.28
ATOM	1653	CG1	VAL	371	66.673	24.429	21.995	1.00	30.02
ATOM	1654	CG2	VAL	371	67.596	23.933	19.746	1.00	32.23
ATOM	1655	C-	VAL	371	69.277	25.417	22.885	1.00	34.44
ATOM	1656	O	VAL	371	68.722	26.331	23.499	1.00	33.35
ATOM	1657	N	THR	372	70.161	24.590	23.443	1.00	33.15
ATOM	1658	CA	THR	372	70.551	24.675	24.847	1.00	32.47
ATOM	1659	CB	THR	372	71.541	23.556	25.207	1.00	32.11
ATOM	1660	OG1	THR	372	70.955	22.288	24.891	1.00	35.33
ATOM	1661	CG2	THR	372	71.894	23.603	26.688	1.00	32.54
ATOM	1662	C	THR	372	71.226	26.020	25.108	1.00	34.49
ATOM	1663	O	THR	372	70.936	26.696	26.099	1.00	34.07
ATOM	1664	N	ASP	373	72.120	26.405	24.202	1.00	32.77
ATOM	1665	CA	ASP	373	72.830	27.671	24.315	1.00	28.08
ATOM	1666	CB	ASP	373	73.803	27.841	23.147	1.00	31.59
ATOM	1667	CG	ASP	373	74.910	26.789	23.142	1.00	37.29
ATOM	1668	OD1	ASP	373	75.170	26.169	24.196	1.00	40.82
ATOM	1669	OD2	ASP	373	75.531	26.586	22.079	1.00	40.81
ATOM	1670	C	ASP	373	71.830	28.821	24.353	1.00	29.21
ATOM	1671	O	ASP	373	71.931	29.709	25.200	1.00	31.85
ATOM	1672	N	LEU	374	70.843	28.775	23.463	1.00	24.71
ATOM	1673	CA	LEU	374	69.813	29.802	23.403	1.00	25.25
ATOM	1674	CB	LEU	374	68.906	29.587	22.188	1.00	25.61
ATOM	1675	CG	LEU	374	69.480	30.084	20.858	1.00	25.51
ATOM	1676	CD1	LEU	374	68.741	29.469	19.677	1.00	23.53
ATOM	1677	CD2	LEU	374	69.405	31.596	20.820	1.00	21.92
ATOM	1678	C	LEU	374	68.994	29.827	24.686	1.00	26.84
ATOM	1679	O	LEU	374	68.591	30.895	25.151	1.00	28.96
ATOM	1680	N	ARG	375	68.746	28.651	25.254	1.00	31.00
ATOM	1681	CA	ARG	375	67.996	28.554	26.502	1.00	32.86
ATOM	1682	CB	ARG	375	67.831	27.090	26.924	1.00	36.80
ATOM	1683	CG	ARG	375	66.861	26.297	26.071	1.00	44.91
ATOM	1684	CD	ARG	375	65.433	26.731	26.338	1.00	58.99
ATOM	1685	NE	ARG	375	64.501	26.210	25.342	1.00	72.26
ATOM	1686	CZ	ARG	375	63.909	25.020	25.404	1.00	77.46
ATOM	1687	NH1	ARG	375	64.147	24.201	26.422	1.00	80.94
ATOM	1688	NH2	ARG	375	63.062	24.657	24.447	1.00	75.58
ATOM	1689	C	ARG	375	68.771	29.317	27.570	1.00	32.27
ATOM	1690	O	ARG	375	68.199	30.125	28.304	1.00	33.75
ATOM	1691	N	MET	376	70.084	29.098	27.602	1.00	32.65
ATOM	1692	CA	MET	376	70.967	29.753	28.560	1.00	35.83
ATOM	1693	CB	MET	376	72.392	29.210	28.434	1.00	39.25
ATOM	1694	CG	MET	376	72.526	27.751	28.839	1.00	54.45
ATOM	1695	SD	MET	376	74.245	27.212	28.944	1.00	73.93
ATOM	1696	CE	MET	376	74.421	26.270	27.434	1.00	67.01

ATOM	1697	C	MET	376	70.960	31.267	28.378	1.00	35.38
ATOM	1698	O	MET	376	70.882	32.015	29.353	1.00	34.73
ATOM	1699	N	ILE	377	71.038	31.716	27.129	1.00	32.51
ATOM	1700	CA	ILE	377	71.016	33.142	26.816	1.00	26.55
ATOM	1701	CB	ILE	377	71.182	33.370	25.299	1.00	24.84
ATOM	1702	CG2	ILE	377	70.817	34.797	24.923	1.00	26.63
ATOM	1703	CG1	ILE	377	72.616	33.038	24.890	1.00	20.66
ATOM	1704	CD1	ILE	377	72.872	33.104	23.409	1.00	20.74
ATOM	1705	C	ILE	377	69.706	33.755	27.313	1.00	25.47
ATOM	1706	O	ILE	377	69.696	34.848	27.881	1.00	29.99
ATOM	1707	N	GLY	378	68.608	33.033	27.127	1.00	25.11
ATOM	1708	CA	GLY	378	67.321	33.522	27.580	1.00	27.82
ATOM	1709	C	GLY	378	67.279	33.613	29.095	1.00	30.90
ATOM	1710	O	GLY	378	66.749	34.579	29.651	1.00	31.19
ATOM	1711	N	ALA	379	67.851	32.611	29.761	1.00	31.62
ATOM	1712	CA	ALA	379	67.896	32.547	31.223	1.00	30.74
ATOM	1713	CB	ALA	379	68.433	31.198	31.671	1.00	30.82
ATOM	1714	C	ALA	379	68.756	33.668	31.801	1.00	30.07
ATOM	1715	O	ALA	379	68.327	34.384	32.708	1.00	31.05
ATOM	1716	N	CYA	380	69.966	33.817	31.273	1.00	29.72
ATOM	1717	CA	CYA	380	70.873	34.866	31.723	1.00	33.36
ATOM	1718	CB	CYA	380	72.201	34.809	30.963	1.00	38.31
ATOM	1719	SG	CYA	380	73.249	33.407	31.386	1.00	50.99
ATOM	1720	AS	CYA	380	74.982	33.655	29.929	1.00	70.37
ATOM	1721	C	CYA	380	70.226	36.232	31.535	1.00	33.40
ATOM	1722	O	CYA	380	70.246	37.062	32.442	1.00	36.41
ATOM	1723	N	HIS	381	69.615	36.456	30.374	1.00	32.55
ATOM	1724	CA	HIS	381	68.965	37.734	30.114	1.00	26.41
ATOM	1725	CB	HIS	381	68.434	37.811	28.681	1.00	20.89
ATOM	1726	CG	HIS	381	67.593	39.023	28.423	1.00	15.78
ATOM	1727	CD2	HIS	381	67.928	40.277	28.041	1.00	12.67
ATOM	1728	ND1	HIS	381	66.226	39.031	28.605	1.00	17.88
ATOM	1729	CE1	HIS	381	65.756	40.239	28.353	1.00	16.27
ATOM	1730	NE2	HIS	381	66.768	41.013	28.008	1.00	17.18
ATOM	1731	C	HIS	381	67.839	38.023	31.102	1.00	26.73
ATOM	1732	O	HIS	381	67.621	39.176	31.464	1.00	30.46
ATOM	1733	N	ALA	382	67.111	36.991	31.521	1.00	26.68
ATOM	1734	CA	ALA	382	66.010	37.176	32.464	1.00	27.90
ATOM	1735	CB	ALA	382	65.237	35.878	32.642	1.00	25.29
ATOM	1736	C	ALA	382	66.511	37.697	33.810	1.00	31.23
ATOM	1737	O	ALA	382	65.927	38.617	34.378	1.00	37.67
ATOM	1738	N	SER	383	67.596	37.114	34.316	1.00	34.15
ATOM	1739	CA	SER	383	68.174	37.550	35.588	1.00	37.23
ATOM	1740	CB	SER	383	69.294	36.605	36.027	1.00	40.21
ATOM	1741	OG	SER	383	68.785	35.324	36.361	1.00	53.99
ATOM									



ATOM	1744	N	ARG	384	69.411	39.171	34.298	1.00	29.95
ATOM	1745	CA	ARG	384	70.000	40.458	33.957	1.00	29.77
ATOM	1746	CB	ARG	384	70.684	40.350	32.594	1.00	30.79
ATOM	1747	CG	ARG	384	71.481	41.558	32.167	1.00	31.34
ATOM	1748	CD	ARG	384	72.781	41.638	32.918	1.00	33.62
ATOM	1749	NE	ARG	384	73.657	42.660	32.358	1.00	41.68
ATOM	1750	CZ	ARG	384	74.584	43.310	33.052	1.00	41.20
ATOM	1751	NH1	ARG	384	74.756	43.047	34.339	1.00	42.11
ATOM	1752	NH2	ARG	384	75.349	44.213	32.455	1.00	37.27
ATOM	1753	C	ARG	384	68.910	41.536	33.911	1.00	35.72
ATOM	1754	O	ARG	384	69.090	42.635	34.439	1.00	41.66
ATOM	1755	N	PHE	385	67.768	41.196	33.318	1.00	34.30
ATOM	1756	CA	PHE	385	66.646	42.119	33.199	1.00	32.40
ATOM	1757	CB	PHE	385	65.527	41.502	32.356	1.00	29.02
ATOM	1758	CG	PHE	385	64.344	42.407	32.163	1.00	26.56
ATOM	1759	CD1	PHE	385	64.317	43.320	31.119	1.00	26.59
ATOM	1760	CD2	PHE	385	63.263	42.355	33.037	1.00	24.69
ATOM	1761	CE1	PHE	385	63.231	44.173	30.947	1.00	31.70
ATOM	1762	CE2	PHE	385	62.174	43.202	32.875	1.00	26.79
ATOM	1763	CZ	PHE	385	62.158	44.115	31.827	1.00	31.59
ATOM	1764	C	PHE	385	66.121	42.492	34.578	1.00	32.98
ATOM	1765	O	PHE	385	65.822	43.659	34.839	1.00	33.91
ATOM	1766	N	LEU	386	66.003	41.499	35.456	1.00	33.91
ATOM	1767	CA	LEU	386	65.533	41.736	36.818	1.00	38.66
ATOM	1768	CB	LEU	386	65.547	40.440	37.633	1.00	43.79
ATOM	1769	CG	LEU	386	64.327	39.521	37.525	1.00	49.81
ATOM	1770	CD1	LEU	386	64.652	38.147	38.099	1.00	51.12
ATOM	1771	CD2	LEU	386	63.135	40.148	38.246	1.00	49.17
ATOM	1772	C	LEU	386	66.445	42.761	37.475	1.00	38.95
ATOM	1773	O	LEU	386	65.979	43.682	38.146	1.00	42.16
ATOM	1774	N	HIS	387	67.745	42.613	37.248	1.00	33.62
ATOM	1775	CA	HIS	387	68.723	43.531	37.808	1.00	39.73
ATOM	1776	CB	HIS	387	70.138	42.980	37.639	1.00	40.71
ATOM	1777	CG	HIS	387	70.403	41.749	38.449	1.00	52.03
ATOM	1778	CD2	HIS	387	69.573	40.967	39.181	1.00	53.85
ATOM	1779	ND1	HIS	387	71.657	41.189	38.566	1.00	54.79
ATOM	1780	CE1	HIS	387	71.590	40.114	39.334	1.00	56.55
ATOM	1781	NE2	HIS	387	70.336	39.958	39.720	1.00	57.48
ATOM	1782	C	HIS	387	68.594	44.913	37.175	1.00	42.08
ATOM	1783	O	HIS	387	68.712	45.926	37.865	1.00	44.12
ATOM	1784	N	MET	388	68.318	44.957	35.874	1.00	42.38
ATOM	1785	CA	MET	388	68.154	46.229	35.175	1.00	38.00
ATOM	1786	CB	MET	388	67.840	46.006	33.692	1.00	40.21
ATOM	1787	CG	MET	388	69.009	45.555	32.829	1.00	41.26
ATOM	1788	SD	MET	388	68.500	45.427	31.089	1.00	45



ATOM	1791	O	MET	388	67.155	48.255	35.997	1.00	38.41
ATOM	1792	N	LYS	389	65.926	46.374	36.144	1.00	39.67
ATOM	1793	CA	LYS	389	64.773	47.036	36.750	1.00	44.96
ATOM	1794	CB	LYS	389	63.570	46.087	36.818	1.00	49.52
ATOM	1795	CG	LYS	389	62.674	46.102	35.588	1.00	56.74
ATOM	1796	CD	LYS	389	62.145	47.509	35.278	1.00	68.05
ATOM	1797	CE	LYS	389	61.287	48.100	36.403	1.00	71.47
ATOM	1798	NZ	LYS	389	60.038	47.330	36.661	1.00	71.98
ATOM	1799	C	LYS	389	65.041	47.604	38.141	1.00	46.60
ATOM	1800	O	LYS	389	64.516	48.661	38.499	1.00	47.25
ATOM	1801	N	VAL	390	65.832	46.893	38.935	1.00	47.15
ATOM	1802	CA	VAL	390	66.129	47.353	40.284	1.00	50.75
ATOM	1803	CB	VAL	390	66.686	46.202	41.182	1.00	50.42
ATOM	1804	CG1	VAL	390	68.095	45.802	40.770	1.00	47.93
ATOM	1805	CG2	VAL	390	66.650	46.612	42.640	1.00	56.67
ATOM	1806	C	VAL	390	67.072	48.558	40.286	1.00	49.82
ATOM	1807	O	VAL	390	66.971	49.426	41.152	1.00	52.44
ATOM	1808	N	GLU	391	67.926	48.651	39.272	1.00	46.14
ATOM	1809	CA	GLU	391	68.888	49.741	39.173	1.00	43.84
ATOM	1810	CB	GLU	391	70.150	49.268	38.449	1.00	41.44
ATOM	1811	CG	GLU	391	70.837	48.074	39.095	1.00	51.12
ATOM	1812	CD	GLU	391	71.218	48.325	40.540	1.00	57.29
ATOM	1813	OE1	GLU	391	71.970	49.287	40.802	1.00	58.15
ATOM	1814	OE2	GLU	391	70.764	47.559	41.416	1.00	62.51
ATOM	1815	C	GLU	391	68.386	51.015	38.501	1.00	45.94
ATOM	1816	O	GLU	391	68.567	52.114	39.033	1.00	51.14
ATOM	1817	N	CYA	392	67.727	50.872	37.354	1.00	45.84
ATOM	1818	CA	CYA	392	67.255	52.029	36.598	1.00	41.60
ATOM	1819	CB	CYA	392	67.681	51.889	35.140	1.00	42.06
ATOM	1820	SG	CYA	392	69.452	52.008	34.968	1.00	44.47
ATOM	1821	AS	CYA	392	69.867	50.812	33.150	1.00	54.22
ATOM	1822	C	CYA	392	65.779	52.395	36.683	1.00	42.27
ATOM	1823	O	CYA	392	64.937	51.564	37.029	1.00	43.91
ATOM	1824	N	PRO	393	65.451	53.674	36.414	1.00	42.79
ATOM	1825	CD	PRO	393	66.384	54.774	36.106	1.00	38.59
ATOM	1826	CA	PRO	393	64.067	54.159	36.459	1.00	44.20
ATOM	1827	CB	PRO	393	64.218	55.667	36.238	1.00	39.88
ATOM	1828	CG	PRO	393	65.487	55.789	35.459	1.00	35.88
ATOM	1829	C	PRO	393	63.178	53.513	35.398	1.00	45.29
ATOM	1830	O	PRO	393	63.600	53.308	34.257	1.00	43.97
ATOM	1831	N	THR	394	61.935	53.238	35.782	1.00	48.20
ATOM	1832	CA	THR	394	60.959	52.607	34.901	1.00	53.71
ATOM	1833	CB	THR	394	59.605	52.429	35.629	1.00	59.59
ATOM	1834	OG1	THR	394	58.690	51.717	34.787	1.00	66.50
ATOM	1835	CG2	THR	394	59.013	53.787	36.004	1.00	61

ATOM	1838	N	GLU	395	61.008	54.664	33.595	1.00	47.65
ATOM	1839	CA	GLU	395	60.845	55.509	32.414	1.00	44.43
ATOM	1840	CB	GLU	395	60.988	56.978	32.804	1.00	43.85
ATOM	1841	C	GLU	395	61.788	55.175	31.250	1.00	42.93
ATOM	1842	O	GLU	395	61.589	55.649	30.129	1.00	41.39
ATOM	1843	N	LEU	396	62.818	54.375	31.517	1.00	39.38
ATOM	1844	CA	LEU	396	63.782	53.989	30.486	1.00	35.70
ATOM	1845	CB	LEU	396	65.185	53.867	31.090	1.00	34.96
ATOM	1846	CG	LEU	396	65.854	55.141	31.609	1.00	36.47
ATOM	1847	CD1	LEU	396	67.234	54.807	32.150	1.00	34.21
ATOM	1848	CD2	LEU	396	65.959	56.164	30.491	1.00	32.74
ATOM	1849	C	LEU	396	63.407	52.671	29.803	1.00	34.60
ATOM	1850	O	LEU	396	64.086	52.223	28.873	1.00	30.36
ATOM	1851	N	PHE	397	62.325	52.059	30.269	1.00	33.02
ATOM	1852	CA	PHE	397	61.868	50.792	29.725	1.00	33.39
ATOM	1853	CB	PHE	397	61.615	49.782	30.852	1.00	34.30
ATOM	1854	CG	PHE	397	62.834	49.439	31.665	1.00	32.62
ATOM	1855	CD1	PHE	397	63.296	50.301	32.654	1.00	32.35
ATOM	1856	CD2	PHE	397	63.504	48.241	31.461	1.00	31.28
ATOM	1857	CE1	PHE	397	64.407	49.976	33.426	1.00	27.01
ATOM	1858	CE2	PHE	397	64.616	47.905	32.229	1.00	33.34
ATOM	1859	CZ	PHE	397	65.067	48.775	33.213	1.00	31.29
ATOM	1860	C	PHE	397	60.580	50.961	28.934	1.00	33.17
ATOM	1861	O	PHE	397	59.540	51.318	29.498	1.00	31.99
ATOM	1862	N	PRO	398	60.636	50.752	27.606	1.00	32.45
ATOM	1863	CD	PRO	398	61.821	50.493	26.768	1.00	28.15
ATOM	1864	CA	PRO	398	59.429	50.885	26.786	1.00	30.02
ATOM	1865	CB	PRO	398	59.921	50.483	25.394	1.00	28.15
ATOM	1866	CG	PRO	398	61.352	50.923	25.397	1.00	24.89
ATOM	1867	C	PRO	398	58.384	49.900	27.326	1.00	28.39
ATOM	1868	O	PRO	398	58.735	48.810	27.789	1.00	28.00
ATOM	1869	N	PRO	399	57.092	50.262	27.267	1.00	32.45
ATOM	1870	CD	PRO	399	56.577	51.511	26.672	1.00	34.93
ATOM	1871	CA	PRO	399	55.989	49.421	27.753	1.00	32.54
ATOM	1872	CB	PRO	399	54.755	50.122	27.188	1.00	34.47
ATOM	1873	CG	PRO	399	55.159	51.564	27.196	1.00	31.37
ATOM	1874	C	PRO	399	56.044	47.946	27.338	1.00	32.18
ATOM	1875	O	PRO	399	55.950	47.054	28.188	1.00	32.58
ATOM	1876	N	LEU	400	56.195	47.689	26.041	1.00	30.15
ATOM	1877	CA	LEU	400	56.259	46.314	25.541	1.00	32.32
ATOM	1878	CB	LEU	400	56.211	46.297	24.011	1.00	28.67
ATOM	1879	CG	LEU	400	56.028	44.927	23.351	1.00	28.77
ATOM	1880	CD1	LEU	400	54.802	44.234	23.919	1.00	22.73
ATOM	1881	CD2	LEU	400	55.897	45.096	21.846	1.00	27.89
ATOM	1882	C	LEU	400	57.496	45.561	26.051	1.00	

ATOM	1885	CA	PHE	401	59.847	45.695	26.710	1.00	32.39
ATOM	1886	CB	PHE	401	60.946	46.769	26.711	1.00	31.38
ATOM	1887	CG	PHE	401	62.290	46.286	27.194	1.00	35.12
ATOM	1888	CD1	PHE	401	62.835	45.089	26.729	1.00	34.68
ATOM	1889	CD2	PHE	401	63.030	47.051	28.097	1.00	34.57
ATOM	1890	CE1	PHE	401	64.100	44.662	27.155	1.00	30.27
ATOM	1891	CE2	PHE	401	64.291	46.635	28.526	1.00	33.57
ATOM	1892	CZ	PHE	401	64.828	45.438	28.054	1.00	35.74
ATOM	1893	C	PHE	401	59.599	45.169	28.129	1.00	32.21
ATOM	1894	O	PHE	401	60.002	44.056	28.478	1.00	33.36
ATOM	1895	N	LEU	402	58.902	45.967	28.929	1.00	31.85
ATOM	1896	CA	LEU	402	58.582	45.602	30.302	1.00	35.06
ATOM	1897	CB	LEU	402	57.948	46.789	31.029	1.00	34.76
ATOM	1898	CG	LEU	402	58.878	47.852	31.591	1.00	33.48
ATOM	1899	CD1	LEU	402	58.060	49.010	32.152	1.00	32.58
ATOM	1900	CD2	LEU	402	59.753	47.217	32.662	1.00	26.27
ATOM	1901	C	LEU	402	57.626	44.426	30.393	1.00	36.80
ATOM	1902	O	LEU	402	57.793	43.545	31.239	1.00	35.43
ATOM	1903	N	GLU	403	56.600	44.443	29.547	1.00	38.50
ATOM	1904	CA	GLU	403	55.581	43.401	29.540	1.00	40.24
ATOM	1905	CB	GLU	403	54.435	43.792	28.605	1.00	44.03
ATOM	1906	CG	GLU	403	53.239	42.850	28.666	1.00	55.53
ATOM	1907	CD	GLU	403	52.180	43.159	27.618	1.00	66.67
ATOM	1908	OE1	GLU	403	52.151	44.299	27.095	1.00	70.81
ATOM	1909	OE2	GLU	403	51.370	42.255	27.315	1.00	73.80
ATOM	1910	C	GLU	403	56.096	42.018	29.162	1.00	38.00
ATOM	1911	O	GLU	403	55.745	41.029	29.805	1.00	38.78
ATOM	1912	N	VAL	404	56.934	41.955	28.132	1.00	37.39
ATOM	1913	CA	VAL	404	57.475	40.686	27.652	1.00	37.05
ATOM	1914	CB	VAL	404	58.180	40.855	26.286	1.00	35.57
ATOM	1915	CG1	VAL	404	58.677	39.513	25.776	1.00	36.85
ATOM	1916	CG2	VAL	404	57.222	41.451	25.287	1.00	42.03
ATOM	1917	C	VAL	404	58.438	40.000	28.609	1.00	38.69
ATOM	1918	O	VAL	404	58.436	38.774	28.727	1.00	40.71
ATOM	1919	N	PHE	405	59.267	40.785	29.286	1.00	39.34
ATOM	1920	CA	PHE	405	60.250	40.221	30.198	1.00	39.33
ATOM	1921	CB	PHE	405	61.620	40.840	29.913	1.00	33.87
ATOM	1922	CG	PHE	405	62.107	40.609	28.509	1.00	32.17
ATOM	1923	CD1	PHE	405	62.355	41.683	27.660	1.00	31.34
ATOM	1924	CD2	PHE	405	62.315	39.317	28.032	1.00	31.98
ATOM	1925	CE1	PHE	405	62.801	41.476	26.352	1.00	30.79
ATOM	1926	CE2	PHE	405	62.759	39.099	26.730	1.00	26.06
ATOM	1927	CZ	PHE	405	63.004	40.182	25.889	1.00	27.98
ATOM	1928	C	PHE	405	59.905	40.322	31.682	1.00	42.64
ATOM	1929	O	PHE	405	60.785	40.188	32.534	1.00	45.10
ATOM	1930	N	GLU	406	58.630	40.536	31.988	1.00	48.95
ATOM	1931	CA	GLU	406	58.181	40.641	33.373	1.00	56.93

ATOM	1932	CB	GLU	406	56.820	41.324	33.432	1.00	56.94
ATOM	1933	C	GLU	406	58.116	39.263	34.040	1.00	61.92
ATOM	1934	O	GLU	406	57.988	38.256	33.308	1.00	67.61
ATOM	1	O1	HOH	501	67.588	36.828	11.225	1.00	27.32
ATOM	2	O1	HOH	502	68.647	41.203	12.940	1.00	39.54
ATOM	3	O1	HOH	503	64.072	40.115	12.407	1.00	32.47
ATOM	4	O1	HOH	504	62.312	39.659	16.075	1.00	17.39
ATOM	5	O1	HOH	505	63.449	46.468	15.530	1.00	30.46
ATOM	6	O1	HOH	506	67.191	15.561	-0.279	1.00	35.96
ATOM	7	O1	HOH	507	67.100	11.855	0.295	1.00	20.00
ATOM	8	O1	HOH	508	61.004	15.510	0.047	1.00	20.00
ATOM	9	O1	HOH	509	59.851	10.761	6.050	1.00	20.00
ATOM	10	O1	HOH	510	57.553	11.824	10.360	1.00	44.63
ATOM	11	O1	HOH	511	54.101	13.545	8.720	1.00	20.00
ATOM	12	O1	HOH	512	55.923	15.916	12.205	1.00	29.31
ATOM	13	O1	HOH	513	50.900	19.934	8.193	1.00	20.00
ATOM	14	O1	HOH	514	50.474	22.912	7.942	1.00	45.34
ATOM	15	O1	HOH	515	49.737	20.631	11.530	1.00	20.00
ATOM	16	O1	HOH	516	50.829	25.467	13.330	1.00	20.00
ATOM	17	O1	HOH	517	53.818	25.833	10.682	1.00	42.12
ATOM	18	O1	HOH	518	52.591	31.216	7.313	1.00	35.55
ATOM	19	O1	HOH	519	58.510	31.667	2.158	1.00	20.00
ATOM	20	O1	HOH	520	58.235	36.751	2.232	1.00	20.00
ATOM	21	O1	HOH	521	62.484	37.992	5.537	1.00	20.00
ATOM	22	O1	HOH	522	68.184	36.969	5.889	1.00	50.08
ATOM	23	O1	HOH	523	66.889	33.781	8.584	1.00	20.00
ATOM	24	O1	HOH	524	67.217	30.836	3.085	1.00	34.44
ATOM	25	O1	HOH	525	64.336	28.325	3.098	1.00	20.00
ATOM	26	O1	HOH	526	67.667	26.625	1.519	1.00	20.00
ATOM	27	O1	HOH	527	76.757	22.883	5.467	1.00	36.94
ATOM	28	O1	HOH	528	72.250	17.936	6.950	1.00	36.00
ATOM	29	O1	HOH	529	71.760	14.791	8.058	1.00	40.18
ATOM	30	O1	HOH	530	72.884	14.751	11.484	1.00	41.44
ATOM	31	O1	HOH	531	69.235	12.986	11.709	1.00	39.38
ATOM	32	O1	HOH	532	69.402	12.036	14.891	1.00	40.68
ATOM	33	O1	HOH	533	64.560	10.910	15.076	1.00	20.00
ATOM	34	O1	HOH	534	63.169	10.413	11.722	1.00	20.00
ATOM	35	O1	HOH	535	66.042	11.455	11.077	1.00	41.05
ATOM	36	O1	HOH	536	76.285	12.458	10.677	1.00	20.00
ATOM	37	O1	HOH	537	81.094	22.520	13.435	1.00	48.70
ATOM	38	O1	HOH	538	80.505	25.457	14.849	1.00	46.30
ATOM	39	O1	HOH	539	77.669	21.932	18.119	1.00	43.79
ATOM	40	O1	HOH	540	77.187	28.903	21.137	1.00	40.22
ATOM	41	O1	HOH	541	76.420	30.760	23.658	1.00	29.63
ATOM	42	O1	HOH	542	83.028	32.743	20.922	1.00	38.14
ATOM	43	O1	HOH	543	82.842	43.133	17.983		



ATOM	45	O1	HOH	545	75.904	32.986	12.256	1.00	34.93
ATOM	46	O1	HOH	546	74.185	29.689	9.761	1.00	38.60
ATOM	47	O1	HOH	547	64.936	20.644	23.365	1.00	36.83
ATOM	48	O1	HOH	548	61.750	22.313	25.288	1.00	34.81
ATOM	49	O1	HOH	549	59.544	21.463	26.162	1.00	20.00
ATOM	50	O1	HOH	550	62.300	27.528	24.386	1.00	35.89
ATOM	51	O1	HOH	551	58.228	29.424	24.603	1.00	25.47
ATOM	52	O1	HOH	552	57.368	32.196	30.527	1.00	45.27
ATOM	53	O1	HOH	553	62.063	36.304	30.245	1.00	42.26
ATOM	54	O1	HOH	554	64.722	36.725	28.906	1.00	24.66
ATOM	55	O1	HOH	555	62.207	35.851	26.642	1.00	30.36
ATOM	56	O1	HOH	556	63.608	33.715	25.707	1.00	42.74
ATOM	57	O1	HOH	557	62.979	38.422	32.977	1.00	49.93
ATOM	58	O1	HOH	558	66.911	33.364	34.901	1.00	50.02
ATOM	59	O1	HOH	559	72.608	29.636	31.674	1.00	37.60
ATOM	60	O1	HOH	560	76.967	40.633	32.514	1.00	44.81
ATOM	61	O1	HOH	561	73.613	41.817	36.847	1.00	31.79
ATOM	62	O1	HOH	562	75.773	46.227	30.514	1.00	29.06
ATOM	63	O1	HOH	563	79.903	46.178	30.800	1.00	41.67
ATOM	64	O1	HOH	564	69.746	51.175	33.564	1.00	20.00
ATOM	65	O1	HOH	565	74.320	52.047	39.438	1.00	20.00
ATOM	66	O1	HOH	566	65.900	53.647	27.404	1.00	40.45
ATOM	67	O1	HOH	567	68.848	53.076	17.895	1.00	39.25
ATOM	68	O1	HOH	568	63.507	48.672	13.581	1.00	43.77
ATOM	69	O1	HOH	569	64.625	46.825	10.331	1.00	20.00
ATOM	70	O1	HOH	570	55.882	41.431	11.148	1.00	20.00
ATOM	71	O1	HOH	571	52.830	43.513	20.032	1.00	35.18
ATOM	72	O1	HOH	572	56.990	49.485	24.052	1.00	37.30
ATOM	73	O1	HOH	573	54.188	47.024	30.900	1.00	52.93
ATOM	74	O1	HOH	574	57.823	44.590	34.025	1.00	53.64
ATOM	75	O1	HOH	575	47.827	29.597	30.690	1.00	37.61
ATOM	76	O1	HOH	576	53.030	24.901	32.732	1.00	45.06
ATOM	77	O1	HOH	577	47.569	19.105	28.647	1.00	38.88
ATOM	78	O1	HOH	578	47.232	20.282	25.561	1.00	20.00
ATOM	79	O1	HOH	579	51.960	14.869	25.534	1.00	49.45
ATOM	80	O1	HOH	580	52.831	23.395	1.634	1.00	20.00
ATOM	81	O1	HOH	581	51.472	22.968	-0.900	1.00	25.10
ATOM	82	O1	HOH	582	77.238	52.503	8.906	1.00	47.05
END									
ATOM	2004	C1	DMT	1	67.320	42.326	18.648	1.00	28.58
ATOM	2005	C2	DMT	1	68.927	43.263	23.318	1.00	29.26
ATOM	2006	C3	DMT	1	67.236	43.583	19.236	1.00	24.54
ATOM	2007	C4	DMT	1	69.268	44.313	24.111	1.00	28.48
ATOM	2008	C5	DMT	1	68.003	43.859	20.363	1.00	28.76
ATOM	2009	C6	DMT	1	68.654	44.389	25.458	1.00	28.16
ATOM	2010	C7	DMT	1	68.811	42.902	20.875	1.00	26.80
ATOM	2011	C8	DMT	1</					





## APPENDIX 4

### TR\_TRIAC.PDB

REMARK

REMARK TR\_triãc full length numbering

REMARK Rfactor 0.236 Rfree 0.241

REMARK Resolution 25. 2.5 all reflections

REMARK

REMARK Three cacodylate-modified cysteines:

REMARK Cys334, Cys380, Cys392

REMARK modeled as free arsenic atoms

REMARK

REMARK conserved polar HOH numbered as in TR\_t3.pdb

REMARK rearrangements start 600

REMARK

REMARK side chain of certain residues modeled as ALA due to poor density;

REMARK however, residue name reflects true residue for clarity

REMARK

REMARK clone obtained from Murray et. al.

REMARK deposited sequence confirmed,

REMARK differing from that reported by Thompson et. al.

REMARK in the following codons:

REMARK 281 Thr - Ala

REMARK 285 Lys - Glu

REMARK identical to that reported by Mitsuhashi et. al.

REMARK gb:RNTRAVI X07409

JRNL AUTH M.B. MURRAY, N.D.ZILZ, N.L.MCCREARY,M.J.MACDONALD

JRNL AUTH 2 H.C.TOWLE

JRNL TITL ISOLATION AND CHARACTERIZATION OF RAT CDNA CLONES  
FOR TWO

JRNL TITL 2 DISTINCT THYROID HORMONE RECPTORS

JRNL REF JBC V. 263 25 1988

JRNL AUTH C.C.THOMPSON, C.WEINBERGER, R.LEBO, R.M.EVANS

JRNL TITL IDENTIFICATION OF A NOVEL THYROID HORMONE RECEPTOR  
EXPRESSED

JRNL TITL 2 IN THE MAMMALIAN CENTRAL NERVOUS SYSTEM

JRNL REF SCIENCE V. 237 1987

JRNL AUTH T.MITSUHASHI,G.TENNYSON,V.NIKODEM

JRNL TITL NUCLEOTIDE SEQUENCE OF NOVEL CDNAS GENERATED BY  
ALTERNATIVE

JRNL TITL 2 SPLICING OF A RAT THYROID HORMONE RECEPTOR GENE  
TRANSCRIPT

JRNL REF NUC. ACIDS. RES. V. 16 12 1988

REMARK

ATOM 1 CB ARG 157 9.880 -24.199 7.196 1.00 57.79

ATOM 2 CG ARG 157 11.380 -24.411 7.340 1.00 57.79

ATOM	3	CD	ARG	157	11.960	-23.602	8.486	1.00	57.79
ATOM	4	NE	ARG	157	11.492	-24.098	9.778	1.00	57.79
ATOM	5	CZ	ARG	157	12.284	-24.379	10.809	1.00	57.79
ATOM	6	NH1	ARG	157	13.598	-24.212	10.714	1.00	57.79
ATOM	7	NH2	ARG	157	11.762	-24.854	11.932	1.00	57.79
ATOM	8	C	ARG	157	7.774	-24.838	5.974	1.00	38.50
ATOM	9	O	ARG	157	7.553	-24.416	4.840	1.00	57.79
ATOM	10	N	ARG	157	9.929	-25.500	5.089	1.00	38.50
ATOM	11	CA	ARG	157	9.183	-25.276	6.360	1.00	38.50
ATOM	12	N	PRO	158	6.802	-24.951	6.895	1.00	23.08
ATOM	13	CD	PRO	158	6.945	-25.424	8.282	1.00	28.38
ATOM	14	CA	PRO	158	5.415	-24.562	6.617	1.00	23.08
ATOM	15	CB	PRO	158	4.704	-24.824	7.948	1.00	28.38
ATOM	16	CG	PRO	158	5.801	-24.735	8.966	1.00	28.38
ATOM	17	C	PRO	158	5.210	-23.124	6.132	1.00	23.08
ATOM	18	O	PRO	158	5.678	-22.167	6.753	1.00	28.38
ATOM	19	N	GLU	159	4.504	-23.000	5.012	1.00	19.26
ATOM	20	CA	GLU	159	4.191	-21.717	4.389	1.00	19.26
ATOM	21	CB	GLU	159	4.022	-21.912	2.878	1.00	24.58
ATOM	22	CG	GLU	159	5.317	-22.009	2.086	1.00	24.58
ATOM	23	CD	GLU	159	5.849	-20.651	1.659	1.00	24.58
ATOM	24	OE1	GLU	159	5.034	-19.722	1.476	1.00	24.58
ATOM	25	OE2	GLU	159	7.080	-20.513	1.490	1.00	24.58
ATOM	26	C	GLU	159	2.879	-21.193	4.968	1.00	19.26
ATOM	27	O	GLU	159	2.152	-21.931	5.636	1.00	24.58
ATOM	28	N	PRO	160	2.579	-19.899	4.765	1.00	17.44
ATOM	29	CD	PRO	160	3.442	-18.817	4.259	1.00	13.94
ATOM	30	CA	PRO	160	1.323	-19.360	5.299	1.00	17.44
ATOM	31	CB	PRO	160	1.414	-17.872	4.956	1.00	13.94
ATOM	32	CG	PRO	160	2.880	-17.604	4.952	1.00	13.94
ATOM	33	C	PRO	160	0.098	-20.006	4.639	1.00	17.44
ATOM	34	O	PRO	160	0.067	-20.207	3.423	1.00	13.94
ATOM	35	N	THR	161	-0.895	-20.352	5.450	1.00	17.00
ATOM	36	CA	THR	161	-2.119	-20.957	4.941	1.00	17.00
ATOM	37	CB	THR	161	-2.958	-21.587	6.086	1.00	20.43
ATOM	38	OG1	THR	161	-3.441	-20.557	6.959	1.00	20.43
ATOM	39	CG2	THR	161	-2.121	-22.576	6.888	1.00	20.43
ATOM	40	C	THR	161	-2.929	-19.843	4.284	1.00	17.00
ATOM	41	O	THR	161	-2.691	-18.660	4.547	1.00	20.43
ATOM	42	N	PRO	162	-3.918	-20.200	3.449	1.00	12.94
ATOM	43	CD	PRO	162	-4.311	-21.559	3.038	1.00	17.56
ATOM	44	CA	PRO	162	-4.743	-19.190	2.780	1.00	12.94
ATOM	45	CB	PRO	162	-5.846	-20.029	2.143	1.00	17.56
ATOM	46	CG	PRO	162	-5.147	-21.303	1.816	1.00	17.56
ATOM	47	C	PRO	162	-5.317	-18.171	3.763	1.00	12.94
ATOM	48	O	PRO	162	-5.305	-16.964	3.503	1.00	17.56
ATOM	49	N	GLU	163	-5.790	-18.668	4.903	1.00	19.45

ATOM	50	CA	GLU	163	-6.374	-17.828	5.943	1.00	19.45
ATOM	51	CB	GLU	163	-6.994	-18.690	7.047	1.00	49.96
ATOM	52	CG	GLU	163	-8.178	-19.558	6.606	1.00	49.96
ATOM	53	CD	GLU	163	-7.782	-20.720	5.697	1.00	49.96
ATOM	54	OE1	GLU	163	-6.735	-21.361	5.951	1.00	49.96
ATOM	55	OE2	GLU	163	-8.527	-20.999	4.731	1.00	49.96
ATOM	56	C	GLU	163	-5.330	-16.897	6.548	1.00	19.45
ATOM	57	O	GLU	163	-5.614	-15.731	6.832	1.00	49.96
ATOM	58	N	GLU	164	-4.120	-17.417	6.734	1.00	22.03
ATOM	59	CA	GLU	164	-3.033	-16.634	7.305	1.00	22.03
ATOM	60	CB	GLU	164	-1.875	-17.541	7.725	1.00	17.15
ATOM	61	CG	GLU	164	-2.198	-18.414	8.937	1.00	17.15
ATOM	62	CD	GLU	164	-1.114	-19.434	9.249	1.00	17.15
ATOM	63	OE1	GLU	164	-0.283	-19.710	8.361	1.00	17.15
ATOM	64	OE2	GLU	164	-1.099	-19.968	10.379	1.00	17.15
ATOM	65	C	GLU	164	-2.559	-15.542	6.354	1.00	22.03
ATOM	66	O	GLU	164	-2.160	-14.470	6.802	1.00	17.15
ATOM	67	N	TRP	165	-2.607	-15.805	5.048	1.00	10.72
ATOM	68	CA	TRP	165	-2.205	-14.803	4.063	1.00	10.72
ATOM	69	CB	TRP	165	-2.223	-15.377	2.644	1.00	2.00
ATOM	70	CG	TRP	165	-0.928	-16.003	2.227	1.00	2.00
ATOM	71	CD2	TRP	165	0.350	-15.358	2.131	1.00	2.00
ATOM	72	CE2	TRP	165	1.275	-16.326	1.685	1.00	2.00
ATOM	73	CE3	TRP	165	0.804	-14.054	2.379	1.00	2.00
ATOM	74	CD1	TRP	165	-0.731	-17.298	1.848	1.00	2.00
ATOM	75	NE1	TRP	165	0.587	-17.500	1.521	1.00	2.00
ATOM	76	CZ2	TRP	165	2.627	-16.036	1.479	1.00	2.00
ATOM	77	CZ3	TRP	165	2.152	-13.764	2.174	1.00	2.00
ATOM	78	CH2	TRP	165	3.046	-14.754	1.729	1.00	2.00
ATOM	79	C	TRP	165	-3.137	-13.601	4.149	1.00	10.72
ATOM	80	O	TRP	165	-2.717	-12.463	3.925	1.00	2.00
ATOM	81	N	ASP	166	-4.408	-13.861	4.441	1.00	14.80
ATOM	82	CA	ASP	166	-5.397	-12.796	4.580	1.00	14.80
ATOM	83	CB	ASP	166	-6.812	-13.370	4.698	1.00	28.74
ATOM	84	CG	ASP	166	-7.298	-13.999	3.403	1.00	28.74
ATOM	85	OD1	ASP	166	-6.909	-13.511	2.320	1.00	28.74
ATOM	86	OD2	ASP	166	-8.071	-14.978	3.466	1.00	28.74
ATOM	87	C	ASP	166	-5.063	-11.981	5.819	1.00	14.80
ATOM	88	O	ASP	166	-5.056	-10.749	5.775	1.00	28.74
ATOM	89	N	LEU	167	-4.745	-12.682	6.906	1.00	11.01
ATOM	90	CA	LEU	167	-4.383	-12.044	8.166	1.00	11.01
ATOM	91	CB	LEU	167	-4.036	-13.103	9.214	1.00	31.53
ATOM	92	CG	LEU	167	-4.672	-12.975	10.601	1.00	31.53
ATOM	93	CD1	LEU	167	-3.806	-13.709	11.619	1.00	31.53
ATOM	94	CD2	LEU	167	-4.820	-11.507	10.989	1.00	31.53
ATOM	95	C	LEU	167	-3.161	-11.159	7.933	1.00	11.01
ATOM	96	O	LEU	167	-3.120	-10.006			

ATOM	97	N	ILE	168	-2.180	-11.714	7.228	1.00	13.18
ATOM	98	CA	ILE	168	-0.937	-11.027	6.900	1.00	13.18
ATOM	99	CB	ILE	168	0.015	-11.968	6.113	1.00	18.30
ATOM	100	CG2	ILE	168	1.118	-11.182	5.414	1.00	18.30
ATOM	101	CG1	ILE	168	0.604	-13.013	7.063	1.00	18.30
ATOM	102	CD1	ILE	168	1.379	-14.111	6.373	1.00	18.30
ATOM	103	C	ILE	168	-1.185	-9.747	6.107	1.00	13.18
ATOM	104	O	ILE	168	-0.637	-8.697	6.437	1.00	18.30
ATOM	105	N	HIS	169	-2.032	-9.831	5.084	1.00	12.99
ATOM	106	CA	HIS	169	-2.342	-8.674	4.245	1.00	12.99
ATOM	107	CB	HIS	169	-3.218	-9.087	3.062	1.00	13.09
ATOM	108	CG	HIS	169	-2.553	-10.045	2.126	1.00	13.09
ATOM	109	CD2	HIS	169	-1.247	-10.223	1.811	1.00	13.09
ATOM	110	ND1	HIS	169	-3.249	-11.000	1.416	1.00	13.09
ATOM	111	CE1	HIS	169	-2.403	-11.728	0.710	1.00	13.09
ATOM	112	NE2	HIS	169	-1.181	-11.277	0.936	1.00	13.09
ATOM	113	C	HIS	169	-3.017	-7.550	5.017	1.00	12.99
ATOM	114	O	HIS	169	-2.680	-6.377	4.839	1.00	13.09
ATOM	115	N	VAL	170	-3.978	-7.909	5.862	1.00	13.36
ATOM	116	CA	VAL	170	-4.696	-6.926	6.664	1.00	13.36
ATOM	117	CB	VAL	170	-5.863	-7.572	7.443	1.00	20.12
ATOM	118	CG1	VAL	170	-6.541	-6.540	8.340	1.00	20.12
ATOM	119	CG2	VAL	170	-6.869	-8.165	6.471	1.00	20.12
ATOM	120	C	VAL	170	-3.741	-6.246	7.639	1.00	13.36
ATOM	121	O	VAL	170	-3.728	-5.019	7.744	1.00	20.12
ATOM	122	N	ALA	171	-2.920	-7.043	8.320	1.00	11.04
ATOM	123	CA	ALA	171	-1.953	-6.515	9.277	1.00	11.04
ATOM	124	CB	ALA	171	-1.249	-7.653	10.005	1.00	13.43
ATOM	125	C	ALA	171	-0.931	-5.613	8.588	1.00	11.04
ATOM	126	O	ALA	171	-0.658	-4.507	9.058	1.00	13.43
ATOM	127	N	THR	172	-0.382	-6.076	7.469	1.00	12.51
ATOM	128	CA	THR	172	0.606	-5.301	6.723	1.00	12.51
ATOM	129	CB	THR	172	1.062	-6.032	5.445	1.00	14.17
ATOM	130	OG1	THR	172	1.548	-7.338	5.782	1.00	14.17
ATOM	131	CG2	THR	172	2.175	-5.255	4.756	1.00	14.17
ATOM	132	C	THR	172	0.045	-3.936	6.337	1.00	12.51
ATOM	133	O	THR	172	0.701	-2.910	6.537	1.00	14.17
ATOM	134	N	GLU	173	-1.178	-3.921	5.815	1.00	17.79
ATOM	135	CA	GLU	173	-1.818	-2.675	5.421	1.00	17.79
ATOM	136	CB	GLU	173	-3.130	-2.946	4.682	1.00	49.44
ATOM	137	CG	GLU	173	-3.823	-1.679	4.171	1.00	49.44
ATOM	138	CD	GLU	173	-2.930	-0.835	3.266	1.00	49.44
ATOM	139	OE1	GLU	173	-2.075	-1.408	2.552	1.00	49.44
ATOM	140	OE2	GLU	173	-3.085	0.404	3.269	1.00	49.44
ATOM	141	C	GLU	173	-2.072	-1.780	6.628	1.00	17.79
ATOM	142	O	GLU	173	-1.854	-0.568	6.557	1.00	49.44
ATOM	143	N	ALA	174	-2.525	-2.375	7.731	1.00	13.



ATOM	144	CA	ALA	174	-2.798	-1.631	8.957	1.00	13.12
ATOM	145	CB	ALA	174	-3.226	-2.576	10.068	1.00	17.51
ATOM	146	C	ALA	174	-1.556	-0.856	9.375	1.00	13.12
ATOM	147	O	ALA	174	-1.634	0.319	9.735	1.00	17.51
ATOM	148	N	HIS	175	-0.409	-1.521	9.317	1.00	12.20
ATOM	149	CA	HIS	175	0.851	-0.895	9.679	1.00	12.20
ATOM	150	CB	HIS	175	1.944	-1.949	9.886	1.00	17.52
ATOM	151	CG	HIS	175	3.302	-1.365	10.136	1.00	17.52
ATOM	152	CD2	HIS	175	3.733	-0.468	11.055	1.00	17.52
ATOM	153	ND1	HIS	175	4.400	-1.679	9.364	1.00	17.52
ATOM	154	CE1	HIS	175	5.447	-0.999	9.793	1.00	17.52
ATOM	155	NE2	HIS	175	5.070	-0.258	10.818	1.00	17.52
ATOM	156	C	HIS	175	1.311	0.133	8.654	1.00	12.20
ATOM	157	O	HIS	175	1.700	1.240	9.024	1.00	17.52
ATOM	158	N	ARG	176	1.291	-0.233	7.375	1.00	12.54
ATOM	159	CA	ARG	176	1.735	0.677	6.328	1.00	12.54
ATOM	160	CB	ARG	176	1.662	0.017	4.950	1.00	50.41
ATOM	161	CG	ARG	176	2.683	-1.088	4.730	1.00	50.41
ATOM	162	CD	ARG	176	2.666	-1.565	3.299	1.00	50.41
ATOM	163	NE	ARG	176	3.682	-2.571	2.989	1.00	50.41
ATOM	164	CZ	ARG	176	3.577	-3.472	2.012	1.00	50.41
ATOM	165	NH1	ARG	176	2.496	-3.513	1.236	1.00	50.41
ATOM	166	NH2	ARG	176	4.536	-4.376	1.841	1.00	50.41
ATOM	167	C	ARG	176	0.972	1.988	6.306	1.00	12.54
ATOM	168	O	ARG	176	1.561	3.040	6.087	1.00	50.41
ATOM	169	N	SER	177	-0.326	1.935	6.581	1.00	24.74
ATOM	170	CA	SER	177	-1.147	3.145	6.584	1.00	24.74
ATOM	171	CB	SER	177	-2.622	2.792	6.414	1.00	21.56
ATOM	172	OG	SER	177	-3.069	1.913	7.436	1.00	21.56
ATOM	173	C	SER	177	-0.960	4.013	7.832	1.00	24.74
ATOM	174	O	SER	177	-1.401	5.159	7.863	1.00	21.56
ATOM	175	N	THR	178	-0.347	3.453	8.870	1.00	17.96
ATOM	176	CA	THR	178	-0.104	4.181	10.115	1.00	17.96
ATOM	177	CB	THR	178	-0.736	3.440	11.323	1.00	19.76
ATOM	178	OG1	THR	178	-0.265	2.091	11.361	1.00	19.76
ATOM	179	CG2	THR	178	-2.253	3.443	11.211	1.00	19.76
ATOM	180	C	THR	178	1.376	4.395	10.382	1.00	17.96
ATOM	181	O	THR	178	1.760	4.880	11.445	1.00	19.76
ATOM	182	N	ASN	179	2.207	4.024	9.417	1.00	25.88
ATOM	183	CA	ASN	179	3.654	4.180	9.546	1.00	25.88
ATOM	184	CB	ASN	179	4.362	2.974	8.943	1.00	44.29
ATOM	185	CG	ASN	179	5.817	2.871	9.368	1.00	44.29
ATOM	186	OD1	ASN	179	6.129	2.768	10.564	1.00	44.29
ATOM	187	ND2	ASN	179	6.719	2.830	8.391	1.00	44.29
ATOM	188	C	ASN	179	4.078	5.458	8.823	1.00	25.88
ATOM	189	O	ASN	179	4.150	5.495	7.590	1.00	44.29
ATOM	190	N	ALA	180	4.332	6.502	9.604	1.00	45.20

ATOM	191	CA	ALA	180	4.740	7.818	9.126	1.00	45.20
ATOM	192	CB	ALA	180	5.026	8.743	10.313	1.00	36.14
ATOM	193	C	ALA	180	5.931	7.808	8.170	1.00	45.20
ATOM	194	O	ALA	180	6.918	7.097	8.372	1.00	36.14
ATOM	195	N	ALA	181	5.784	8.552	7.080	1.00	44.05
ATOM	196	CA	ALA	181	6.834	8.661	6.072	1.00	44.05
ATOM	197	CB	ALA	181	8.170	9.116	6.722	1.00	50.21
ATOM	198	C	ALA	181	7.069	7.427	5.196	1.00	44.05
ATOM	199	O	ALA	181	7.663	7.550	4.118	1.00	50.21
ATOM	200	N	GLY	182	6.567	6.268	5.622	1.00	39.06
ATOM	201	CA	GLY	182	6.756	5.040	4.867	1.00	39.06
ATOM	202	C	GLY	182	8.202	4.769	4.482	1.00	39.06
ATOM	203	O	GLY	182	9.096	4.785	5.334	1.00	48.58
ATOM	204	N	SER	183	8.438	4.564	3.189	1.00	64.55
ATOM	205	CA	SER	183	9.781	4.270	2.693	1.00	64.55
ATOM	206	CB	SER	183	9.690	3.402	1.430	1.00	67.68
ATOM	207	OG	SER	183	8.822	3.978	0.467	1.00	67.68
ATOM	208	C	SER	183	10.643	5.510	2.437	1.00	64.55
ATOM	209	O	SER	183	11.839	5.407	2.158	1.00	67.68
ATOM	210	N	HIS	184	10.035	6.683	2.579	1.00	52.73
ATOM	211	CA	HIS	184	10.725	7.953	2.352	1.00	52.73
ATOM	212	CB	HIS	184	9.772	8.955	1.698	1.00	44.77
ATOM	213	C	HIS	184	11.364	8.582	3.595	1.00	52.73
ATOM	214	O	HIS	184	11.837	9.722	3.540	1.00	44.77
ATOM	215	N	TRP	185	11.420	7.842	4.699	1.00	54.14
ATOM	216	CA	TRP	185	11.977	8.389	5.940	1.00	54.14
ATOM	217	CB	TRP	185	11.813	7.395	7.104	1.00	40.24
ATOM	218	CG	TRP	185	12.605	6.123	6.991	1.00	40.24
ATOM	219	CD2	TRP	185	13.894	5.873	7.551	1.00	40.24
ATOM	220	CE2	TRP	185	14.245	4.543	7.221	1.00	40.24
ATOM	221	CE3	TRP	185	14.791	6.641	8.300	1.00	40.24
ATOM	222	CD1	TRP	185	12.227	4.973	6.359	1.00	40.24
ATOM	223	NE1	TRP	185	13.210	4.015	6.496	1.00	40.24
ATOM	224	CZ2	TRP	185	15.461	3.968	7.619	1.00	40.24
ATOM	225	CZ3	TRP	185	15.996	6.073	8.696	1.00	40.24
ATOM	226	CH2	TRP	185	16.319	4.747	8.353	1.00	40.24
ATOM	227	C	TRP	185	13.432	8.870	5.819	1.00	54.14
ATOM	228	O	TRP	185	13.759	10.008	6.168	1.00	40.24
ATOM	229	N	LYS	186	14.277	8.032	5.232	1.00	43.72
ATOM	230	CA	LYS	186	15.694	8.329	5.035	1.00	43.72
ATOM	231	CB	LYS	186	16.353	7.168	4.282	1.00	64.14
ATOM	232	CG	LYS	186	17.830	7.355	3.945	1.00	64.14
ATOM	233	CD	LYS	186	18.758	7.175	5.139	1.00	64.14
ATOM	234	CE	LYS	186	20.195	7.060	4.652	1.00	64.14
ATOM	235	NZ	LYS	186	20.348	5.838	3.805	1.00	64.14
ATOM	236	C	LYS	186	15.900	9.634	4.263	1.00	43.72
ATOM	237	O	LYS	186	16.948				

ATOM	238	N	GLN	187	14.892	10.032	3.491	1.00	58.06
ATOM	239	CA	GLN	187	14.958	11.244	2.682	1.00	58.06
ATOM	240	CB	GLN	187	14.288	10.997	1.321	1.00	74.68
ATOM	241	CG	GLN	187	14.639	9.662	0.667	1.00	74.68
ATOM	242	CD	GLN	187	16.133	9.397	0.607	1.00	74.68
ATOM	243	OE1	GLN	187	16.926	10.312	0.381	1.00	74.68
ATOM	244	NE2	GLN	187	16.528	8.156	0.855	1.00	74.68
ATOM	245	C	GLN	187	14.322	12.466	3.342	1.00	58.06
ATOM	246	O	GLN	187	14.897	13.551	3.358	1.00	74.68
ATOM	247	N	ARG	188	13.117	12.280	3.866	1.00	54.11
ATOM	248	CA	ARG	188	12.363	13.360	4.505	1.00	54.11
ATOM	249	CB	ARG	188	10.889	13.115	4.334	1.00	53.33
ATOM	250	C	ARG	188	12.654	13.626	5.977	1.00	54.11
ATOM	251	O	ARG	188	11.879	14.298	6.659	1.00	53.33
ATOM	252	N	ARG	189	13.754	13.090	6.473	1.00	39.52
ATOM	253	CA	ARG	189	14.089	13.271	7.875	1.00	39.52
ATOM	254	CB	ARG	189	14.594	11.959	8.482	1.00	60.85
ATOM	255	CG	ARG	189	15.969	11.555	7.991	1.00	60.85
ATOM	256	CD	ARG	189	16.442	10.298	8.693	1.00	60.85
ATOM	257	NE	ARG	189	17.833	9.963	8.385	1.00	60.85
ATOM	258	CZ	ARG	189	18.627	9.261	9.190	1.00	60.85
ATOM	259	NH1	ARG	189	18.178	8.805	10.356	1.00	60.85
ATOM	260	NH2	ARG	189	19.882	9.021	8.841	1.00	60.85
ATOM	261	C	ARG	189	15.109	14.378	8.109	1.00	39.52
ATOM	262	O	ARG	189	16.037	14.565	7.320	1.00	60.85
ATOM	263	N	LYS	190	14.934	15.100	9.212	1.00	44.13
ATOM	264	CA	LYS	190	15.834	16.183	9.586	1.00	44.13
ATOM	265	CB	LYS	190	15.068	17.500	9.680	1.00	45.33
ATOM	266	C	LYS	190	16.472	15.846	10.928	1.00	44.13
ATOM	267	O	LYS	190	15.827	15.272	11.805	1.00	45.33
ATOM	268	N	PHE	191	17.748	16.184	11.067	1.00	35.64
ATOM	269	CA	PHE	191	18.489	15.928	12.291	1.00	35.64
ATOM	270	CB	PHE	191	19.993	16.008	12.025	1.00	53.94
ATOM	271	CG	PHE	191	20.550	14.827	11.286	1.00	53.94
ATOM	272	CD1	PHE	191	20.209	14.596	9.958	1.00	53.94
ATOM	273	CD2	PHE	191	21.430	13.949	11.915	1.00	53.94
ATOM	274	CE1	PHE	191	20.735	13.510	9.265	1.00	53.94
ATOM	275	CE2	PHE	191	21.964	12.859	11.230	1.00	53.94
ATOM	276	CZ	PHE	191	21.615	12.639	9.900	1.00	53.94
ATOM	277	C	PHE	191	18.135	16.928	13.384	1.00	35.64
ATOM	278	O	PHE	191	17.997	18.127	13.120	1.00	53.94
ATOM	279	N	LEU	192	17.978	16.439	14.610	1.00	44.53
ATOM	280	CA	LEU	192	17.683	17.315	15.736	1.00	44.53
ATOM	281	CB	LEU	192	17.326	16.493	16.980	1.00	22.94
ATOM	282	CG	LEU	192	16.931	17.259	18.246	1.00	22.94
ATOM	283	CD1	LEU	192	15.568	17.906	18.064		

ATOM	285	C	LEU	192	18.974	18.101	15.980	1.00	44.53
ATOM	286	O	LEU	192	20.049	17.507	16.129	1.00	22.94
ATOM	287	N	PRO	193	18.895	19.444	15.977	1.00	34.26
ATOM	288	CD	PRO	193	17.670	20.241	15.781	1.00	46.23
ATOM	289	CA	PRO	193	20.058	20.311	16.198	1.00	34.26
ATOM	290	CB	PRO	193	19.417	21.670	16.465	1.00	46.23
ATOM	291	CG	PRO	193	18.213	21.641	15.579	1.00	46.23
ATOM	292	C	PRO	193	20.917	19.844	17.372	1.00	34.26
ATOM	293	O	PRO	193	20.413	19.614	18.471	1.00	46.23
ATOM	294	N	ASP	194	22.217	19.716	17.125	1.00	42.67
ATOM	295	CA	ASP	194	23.174	19.254	18.128	1.00	42.67
ATOM	296	CB	ASP	194	24.583	19.226	17.536	1.00	68.50
ATOM	297	CG	ASP	194	24.731	18.185	16.450	1.00	68.50
ATOM	298	OD1	ASP	194	25.066	17.027	16.782	1.00	68.50
ATOM	299	OD2	ASP	194	24.498	18.518	15.269	1.00	68.50
ATOM	300	C	ASP	194	23.187	20.003	19.457	1.00	42.67
ATOM	301	O	ASP	194	23.545	19.432	20.486	1.00	68.50
ATOM	302	N	ASP	195	22.817	21.280	19.438	1.00	47.52
ATOM	303	CA	ASP	195	22.793	22.070	20.666	1.00	47.52
ATOM	304	CB	ASP	195	22.586	23.559	20.351	1.00	85.02
ATOM	305	CG	ASP	195	21.327	23.824	19.537	1.00	85.02
ATOM	306	OD1	ASP	195	20.291	24.188	20.138	1.00	85.02
ATOM	307	OD2	ASP	195	21.377	23.683	18.294	1.00	85.02
ATOM	308	C	ASP	195	21.715	21.561	21.627	1.00	47.52
ATOM	309	O	ASP	195	21.762	21.826	22.831	1.00	85.02
ATOM	310	N	ILE	196	20.760	20.810	21.089	1.00	44.54
ATOM	311	CA	ILE	196	19.663	20.259	21.875	1.00	44.54
ATOM	312	CB	ILE	196	18.379	20.137	21.023	1.00	39.66
ATOM	313	CG2	ILE	196	17.223	19.627	21.874	1.00	39.66
ATOM	314	CG1	ILE	196	18.031	21.496	20.407	1.00	39.66
ATOM	315	CD1	ILE	196	16.816	21.475	19.503	1.00	39.66
ATOM	316	C	ILE	196	20.030	18.882	22.420	1.00	44.54
ATOM	317	O	ILE	196	20.582	18.046	21.705	1.00	39.66
ATOM	318	N	GLY	197	19.714	18.652	23.690	1.00	42.85
ATOM	319	CA	GLY	197	20.006	17.372	24.307	1.00	42.85
ATOM	320	C	GLY	197	21.371	17.285	24.956	1.00	42.85
ATOM	321	O	GLY	197	21.815	16.198	25.318	1.00	40.22
ATOM	322	N	GLN	198	22.029	18.425	25.137	1.00	53.07
ATOM	323	CA	GLN	198	23.351	18.444	25.754	1.00	53.07
ATOM	324	CB	GLN	198	24.357	19.103	24.810	1.00	44.23
ATOM	325	C	GLN	198	23.344	19.153	27.110	1.00	53.07
ATOM	326	O	GLN	198	24.396	19.545	27.616	1.00	44.23
ATOM	327	N	SER	199	22.170	19.244	27.729	1.00	35.30
ATOM	328	CA	SER	199	22.037	19.918	29.019	1.00	35.30
ATOM	329	CB	SER	199	21.472	21.328	28.806	1.00	58.72
ATOM	330	OG	SER	199	22.093				



ATOM	332	O	SER	199	20.135	19.681	30.482	1.00	58.72
ATOM	333	N	PRO	200	21.544	17.928	30.387	1.00	34.70
ATOM	334	CD	PRO	200	22.656	17.108	29.872	1.00	38.71
ATOM	335	CA	PRO	200	20.740	17.184	31.362	1.00	34.70
ATOM	336	CB	PRO	200	21.311	15.769	31.266	1.00	38.71
ATOM	337	CG	PRO	200	22.737	15.992	30.878	1.00	38.71
ATOM	338	C	PRO	200	20.923	17.784	32.759	1.00	34.70
ATOM	339	O	PRO	200	22.006	17.692	33.341	1.00	38.71
ATOM	340	N	ILE	201	19.876	18.413	33.286	1.00	42.94
ATOM	341	CA	ILE	201	19.961	19.041	34.604	1.00	42.94
ATOM	342	CB	ILE	201	20.059	20.582	34.491	1.00	51.32
ATOM	343	CG2	ILE	201	21.468	20.991	34.078	1.00	51.32
ATOM	344	CG1	ILE	201	19.009	21.111	33.510	1.00	51.32
ATOM	345	CD1	ILE	201	19.169	22.582	33.164	1.00	51.32
ATOM	346	C	ILE	201	18.871	18.676	35.610	1.00	42.94
ATOM	347	O	ILE	201	19.049	18.875	36.814	1.00	51.32
ATOM	348	N	VAL	202	17.737	18.172	35.133	1.00	50.33
ATOM	349	CA	VAL	202	16.661	17.787	36.043	1.00	50.33
ATOM	350	CB	VAL	202	15.296	17.722	35.326	1.00	36.59
ATOM	351	CG1	VAL	202	14.202	17.311	36.304	1.00	36.59
ATOM	352	CG2	VAL	202	14.968	19.074	34.714	1.00	36.59
ATOM	353	C	VAL	202	17.007	16.435	36.665	1.00	50.33
ATOM	354	O	VAL	202	17.335	15.481	35.955	1.00	36.59
ATOM	355	N	SER	203	16.960	16.375	37.991	1.00	49.46
ATOM	356	CA	SER	203	17.289	15.166	38.736	1.00	49.46
ATOM	357	CB	SER	203	17.298	15.467	40.241	1.00	64.20
ATOM	358	OG	SER	203	17.673	14.330	41.003	1.00	64.20
ATOM	359	C	SER	203	16.356	13.992	38.463	1.00	49.46
ATOM	360	O	SER	203	15.147	14.166	38.310	1.00	64.20
ATOM	361	N	MET	204	16.944	12.800	38.419	1.00	41.99
ATOM	362	CA	MET	204	16.223	11.551	38.205	1.00	41.99
ATOM	363	CB	MET	204	16.320	11.096	36.746	1.00	48.64
ATOM	364	CG	MET	204	15.470	11.895	35.771	1.00	48.64
ATOM	365	SD	MET	204	13.702	11.783	36.114	1.00	48.64
ATOM	366	CE	MET	204	13.284	10.257	35.264	1.00	48.64
ATOM	367	C	MET	204	16.900	10.528	39.109	1.00	41.99
ATOM	368	O	MET	204	18.127	10.417	39.121	1.00	48.64
ATOM	369	N	PRO	205	16.108	9.754	39.869	1.00	38.42
ATOM	370	CD	PRO	205	14.633	9.815	39.866	1.00	52.20
ATOM	371	CA	PRO	205	16.586	8.724	40.797	1.00	38.42
ATOM	372	CB	PRO	205	15.334	7.888	41.041	1.00	52.20
ATOM	373	CG	PRO	205	14.254	8.919	41.028	1.00	52.20
ATOM	374	C	PRO	205	17.769	7.858	40.340	1.00	38.42
ATOM	375	O	PRO	205	18.724	7.675	41.092	1.00	52.20
ATOM	376	N	ASP	206	17.720	7.349	39.111	1.00	49.06
ATOM	377	CA	ASP	206	18.791	6.490	38.601		



ATOM	379	CG	ASP	206	17.690	6.450	36.305	1.00	74.42
ATOM	380	OD1	ASP	206	18.397	7.335	35.770	1.00	74.42
ATOM	381	OD2	ASP	206	16.516	6.199	35.948	1.00	74.42
ATOM	382	C	ASP	206	20.106	7.177	38.214	1.00	49.06
ATOM	383	O	ASP	206	21.069	6.506	37.838	1.00	74.42
ATOM	384	N <sup>+</sup>	GLY	207	20.139	8.505	38.272	1.00	42.48
ATOM	385	CA	GLY	207	21.355	9.225	37.928	1.00	42.48
ATOM	386	C	GLY	207	21.330	9.965	36.601	1.00	42.48
ATOM	387	O	GLY	207	21.890	11.058	36.494	1.00	42.50
ATOM	388	N	ASP	208	20.725	9.365	35.581	1.00	46.70
ATOM	389	CA	ASP	208	20.636	9.999	34.266	1.00	46.70
ATOM	390	CB	ASP	208	20.162	8.994	33.212	1.00	61.56
ATOM	391	CG	ASP	208	21.143	7.856	33.006	1.00	61.56
ATOM	392	OD1	ASP	208	20.723	6.684	33.122	1.00	61.56
ATOM	393	OD2	ASP	208	22.330	8.134	32.724	1.00	61.56
ATOM	394	C	ASP	208	19.666	11.176	34.339	1.00	46.70
ATOM	395	O	ASP	208	18.462	10.983	34.506	1.00	61.56
ATOM	396	N	LYS	209	20.200	12.389	34.238	1.00	41.30
ATOM	397	CA	LYS	209	19.389	13.602	34.308	1.00	41.30
ATOM	398	CB	LYS	209	20.254	14.782	34.732	1.00	41.38
ATOM	399	C	LYS	209	18.657	13.916	33.004	1.00	41.30
ATOM	400	O	LYS	209	19.052	13.458	31.930	1.00	41.38
ATOM	401	N	VAL	210	17.603	14.723	33.109	1.00	43.36
ATOM	402	CA	VAL	210	16.792	15.107	31.954	1.00	43.36
ATOM	403	CB	VAL	210	15.275	15.014	32.282	1.00	30.23
ATOM	404	CG1	VAL	210	14.440	15.358	31.055	1.00	30.23
ATOM	405	CG2	VAL	210	14.923	13.624	32.782	1.00	30.23
ATOM	406	C	VAL	210	17.088	16.522	31.442	1.00	43.36
ATOM	407	O	VAL	210	17.395	17.430	32.221	1.00	30.23
ATOM	408	N	ASP	211	17.004	16.685	30.125	1.00	27.49
ATOM	409	CA	ASP	211	17.217	17.966	29.458	1.00	27.49
ATOM	410	CB	ASP	211	18.073	17.765	28.198	1.00	30.75
ATOM	411	CG	ASP	211	18.360	19.068	27.447	1.00	30.75
ATOM	412	OD1	ASP	211	19.473	19.196	26.900	1.00	30.75
ATOM	413	OD2	ASP	211	17.484	19.955	27.370	1.00	30.75
ATOM	414	C	ASP	211	15.819	18.445	29.073	1.00	27.49
ATOM	415	O	ASP	211	15.197	17.892	28.166	1.00	30.75
ATOM	416	N	LEU	212	15.343	19.488	29.745	1.00	31.99
ATOM	417	CA	LEU	212	14.013	20.042	29.492	1.00	31.99
ATOM	418	CB	LEU	212	13.778	21.274	30.369	1.00	35.19
ATOM	419	CG	LEU	212	13.606	20.997	31.864	1.00	35.19
ATOM	420	CD1	LEU	212	13.621	22.298	32.652	1.00	35.19
ATOM	421	CD2	LEU	212	12.309	20.237	32.098	1.00	35.19
ATOM	422	C	LEU	212	13.713	20.377	28.032	1.00	31.99
ATOM	423	O	LEU	212	12.625	20.083	27.539	1.00	35.19
ATOM	424	N	GLU	213	14.672				

ATOM	426	CB	GLU	213	15.623	22.209	25.428	1.00	62.21
ATOM	427	CG	GLU	213	15.434	22.707	23.997	1.00	62.21
ATOM	428	CD	GLU	213	16.651	23.440	23.446	1.00	62.21
ATOM	429	OE1	GLU	213	17.778	23.214	23.945	1.00	62.21
ATOM	430	OE2	GLU	213	16.478	24.237	22.498	1.00	62.21
ATOM	431	C	GLU	213	14.317	20.104	25.067	1.00	28.70
ATOM	432	O	GLU	213	13.403	20.024	24.247	1.00	62.21
ATOM	433	N	ALA	214	15.201	19.130	25.262	1.00	28.17
ATOM	434	CA	ALA	214	15.162	17.890	24.494	1.00	28.17
ATOM	435	CB	ALA	214	16.330	16.998	24.872	1.00	42.74
ATOM	436	C	ALA	214	13.844	17.176	24.759	1.00	28.17
ATOM	437	O	ALA	214	13.174	16.726	23.829	1.00	42.74
ATOM	438	N	PHE	215	13.468	17.104	26.032	1.00	21.66
ATOM	439	CA	PHE	215	12.222	16.471	26.444	1.00	21.66
ATOM	440	CB	PHE	215	12.033	16.628	27.958	1.00	28.76
ATOM	441	CG	PHE	215	10.751	16.038	28.481	1.00	28.76
ATOM	442	CD1	PHE	215	10.675	14.689	28.815	1.00	28.76
ATOM	443	CD2	PHE	215	9.623	16.835	28.653	1.00	28.76
ATOM	444	CE1	PHE	215	9.493	14.143	29.315	1.00	28.76
ATOM	445	CE2	PHE	215	8.438	16.300	29.150	1.00	28.76
ATOM	446	CZ	PHE	215	8.373	14.951	29.482	1.00	28.76
ATOM	447	C	PHE	215	11.068	17.132	25.696	1.00	21.66
ATOM	448	O	PHE	215	10.215	16.451	25.122	1.00	28.76
ATOM	449	N	SER	216	11.073	18.462	25.680	1.00	28.03
ATOM	450	CA	SER	216	10.043	19.242	25.007	1.00	28.03
ATOM	451	CB	SER	216	10.349	20.734	25.146	1.00	33.85
ATOM	452	OG	SER	216	9.300	21.529	24.624	1.00	33.85
ATOM	453	C	SER	216	9.945	18.857	23.532	1.00	28.03
ATOM	454	O	SER	216	8.852	18.613	23.019	1.00	33.85
ATOM	455	N	GLU	217	11.092	18.761	22.868	1.00	28.84
ATOM	456	CA	GLU	217	11.138	18.402	21.454	1.00	28.84
ATOM	457	CB	GLU	217	12.581	18.420	20.943	1.00	47.68
ATOM	458	CG	GLU	217	13.174	19.815	20.811	1.00	47.68
ATOM	459	CD	GLU	217	12.405	20.684	19.829	1.00	47.68
ATOM	460	OE1	GLU	217	11.660	21.581	20.281	1.00	47.68
ATOM	461	OE2	GLU	217	12.542	20.465	18.606	1.00	47.68
ATOM	462	C	GLU	217	10.505	17.044	21.179	1.00	28.84
ATOM	463	O	GLU	217	9.751	16.886	20.217	1.00	47.68
ATOM	464	N	PHE	218	10.799	16.071	22.036	1.00	21.49
ATOM	465	CA	PHE	218	10.259	14.725	21.883	1.00	21.49
ATOM	466	CB	PHE	218	11.020	13.746	22.781	1.00	24.12
ATOM	467	CG	PHE	218	12.489	13.652	22.464	1.00	24.12
ATOM	468	CD1	PHE	218	13.431	13.554	23.481	1.00	24.12
ATOM	469	CD2	PHE	218	12.932	13.677	21.144	1.00	24.12
ATOM	470	CE1	PHE	218	14.793	13.484	23.187	1.00	24.12
ATOM	471	CE2	PHE	218	1				

ATOM	473	C	PHE	218	8.765	14.675	22.176	1.00	21.49
ATOM	474	O	PHE	218	7.985	14.166	21.369	1.00	24.12
ATOM	475	N	THR	219	8.358	15.227	23.312	1.00	20.07
ATOM	476	CA	THR	219	6.949	15.231	23.685	1.00	20.07
ATOM	477	CB	THR	219	6.741	15.766	25.118	1.00	28.98
ATOM	478	OG1	THR	219	7.418	17.021	25.274	1.00	28.98
ATOM	479	CG2	THR	219	7.275	14.767	26.132	1.00	28.98
ATOM	480	C	THR	219	6.080	16.011	22.696	1.00	20.07
ATOM	481	O	THR	219	4.914	15.670	22.482	1.00	28.98
ATOM	482	N	LYS	220	6.662	17.022	22.060	1.00	25.35
ATOM	483	CA	LYS	220	5.943	17.840	21.088	1.00	25.35
ATOM	484	CB	LYS	220	6.842	18.965	20.577	1.00	29.07
ATOM	485	C	LYS	220	5.414	17.015	19.916	1.00	25.35
ATOM	486	O	LYS	220	4.376	17.343	19.339	1.00	29.07
ATOM	487	N	ILE	221	6.122	15.943	19.569	1.00	31.43
ATOM	488	CA	ILE	221	5.708	15.089	18.458	1.00	31.43
ATOM	489	CB	ILE	221	6.842	14.915	17.413	1.00	25.19
ATOM	490	CG2	ILE	221	7.240	16.264	16.838	1.00	25.19
ATOM	491	CG1	ILE	221	8.050	14.215	18.043	1.00	25.19
ATOM	492	CD1	ILE	221	9.113	13.799	17.044	1.00	25.19
ATOM	493	C	ILE	221	5.240	13.700	18.892	1.00	31.43
ATOM	494	O	ILE	221	4.930	12.857	18.046	1.00	25.19
ATOM	495	N	ILE	222	5.129	13.474	20.198	1.00	24.41
ATOM	496	CA	ILE	222	4.720	12.162	20.687	1.00	24.41
ATOM	497	CB	ILE	222	5.189	11.916	22.147	1.00	27.10
ATOM	498	CG2	ILE	222	4.221	12.545	23.145	1.00	27.10
ATOM	499	CG1	ILE	222	5.302	10.410	22.400	1.00	27.10
ATOM	500	CD1	ILE	222	6.062	10.053	23.646	1.00	27.10
ATOM	501	C	ILE	222	3.231	11.845	20.541	1.00	24.41
ATOM	502	O	ILE	222	2.864	10.691	20.307	1.00	27.10
ATOM	503	N	THR	223	2.378	12.861	20.642	1.00	33.16
ATOM	504	CA	THR	223	0.936	12.653	20.520	1.00	33.16
ATOM	505	CB	THR	223	0.150	13.974	20.721	1.00	36.84
ATOM	506	OG1	THR	223	0.352	14.442	22.063	1.00	36.84
ATOM	507	CG2	THR	223	-1.346	13.764	20.484	1.00	36.84
ATOM	508	C	THR	223	0.536	11.954	19.212	1.00	33.16
ATOM	509	O	THR	223	-0.156	10.932	19.242	1.00	36.84
ATOM	510	N	PRO	224	0.968	12.482	18.048	1.00	18.75
ATOM	511	CD	PRO	224	1.691	13.735	17.770	1.00	26.12
ATOM	512	CA	PRO	224	0.590	11.805	16.802	1.00	18.75
ATOM	513	CB	PRO	224	1.117	12.747	15.715	1.00	26.12
ATOM	514	CG	PRO	224	2.221	13.497	16.386	1.00	26.12
ATOM	515	C	PRO	224	1.200	10.402	16.701	1.00	18.75
ATOM	516	O	PRO	224	0.606	9.502	16.101	1.00	26.12
ATOM	517	N	ALA	225	2.368	10.213	17.312	1.00	12.19
ATOM	518	CA	ALA	225	3.040	8.916	17.300	1.00	12.19
ATOM									

ATOM	520	C	ALA	225	2.187	7.881	18.030	1.00	12.19
ATOM	521	O	ALA	225	1.998	6.764	17.545	1.00	20.39
ATOM	522	N	ILE	226	1.645	8.271	19.179	1.00	14.61
ATOM	523	CA	ILE	226	0.798	7.385	19.971	1.00	14.61
ATOM	524	CB	ILE	226	0.450	8.025	21.332	1.00	16.10
ATOM	525	CG2	ILE	226	-0.508	7.132	22.108	1.00	16.10
ATOM	526	CG1	ILE	226	1.729	8.293	22.132	1.00	16.10
ATOM	527	CD1	ILE	226	1.509	9.113	23.387	1.00	16.10
ATOM	528	C	ILE	226	-0.499	7.094	19.213	1.00	14.61
ATOM	529	O	ILE	226	-0.986	5.961	19.200	1.00	16.10
ATOM	530	N	THR	227	-1.042	8.123	18.569	1.00	15.93
ATOM	531	CA	THR	227	-2.278	7.997	17.800	1.00	15.93
ATOM	532	CB	THR	227	-2.706	9.360	17.207	1.00	22.37
ATOM	533	OG1	THR	227	-2.890	10.301	18.273	1.00	22.37
ATOM	534	CG2	THR	227	-4.014	9.232	16.434	1.00	22.37
ATOM	535	C	THR	227	-2.149	6.964	16.680	1.00	15.93
ATOM	536	O	THR	227	-3.091	6.217	16.402	1.00	22.37
ATOM	537	N	ARG	228	-0.982	6.916	16.045	1.00	14.49
ATOM	538	CA	ARG	228	-0.750	5.956	14.975	1.00	14.49
ATOM	539	CB	ARG	228	0.602	6.188	14.307	1.00	33.87
ATOM	540	CG	ARG	228	0.701	7.482	13.540	1.00	33.87
ATOM	541	CD	ARG	228	2.053	7.572	12.868	1.00	33.87
ATOM	542	NE	ARG	228	2.510	8.952	12.793	1.00	33.87
ATOM	543	CZ	ARG	228	3.551	9.431	13.469	1.00	33.87
ATOM	544	NH1	ARG	228	4.256	8.634	14.270	1.00	33.87
ATOM	545	NH2	ARG	228	3.864	10.716	13.374	1.00	33.87
ATOM	546	C	ARG	228	-0.813	4.531	15.516	1.00	14.49
ATOM	547	O	ARG	228	-1.309	3.632	14.839	1.00	33.87
ATOM	548	N	VAL	229	-0.313	4.327	16.735	1.00	14.80
ATOM	549	CA	VAL	229	-0.333	3.002	17.352	1.00	14.80
ATOM	550	CB	VAL	229	0.456	2.979	18.683	1.00	13.78
ATOM	551	CG1	VAL	229	0.339	1.612	19.350	1.00	13.78
ATOM	552	CG2	VAL	229	1.915	3.312	18.430	1.00	13.78
ATOM	553	C	VAL	229	-1.788	2.602	17.591	1.00	14.80
ATOM	554	O	VAL	229	-2.185	1.465	17.323	1.00	13.78
ATOM	555	N	VAL	230	-2.588	3.561	18.047	1.00	9.33
ATOM	556	CA	VAL	230	-4.005	3.327	18.292	1.00	9.33
ATOM	557	CB	VAL	230	-4.679	4.564	18.909	1.00	16.07
ATOM	558	CG1	VAL	230	-6.168	4.319	19.076	1.00	16.07
ATOM	559	CG2	VAL	230	-4.038	4.896	20.253	1.00	16.07
ATOM	560	C	VAL	230	-4.700	2.982	16.981	1.00	9.33
ATOM	561	O	VAL	230	-5.504	2.049	16.929	1.00	16.07
ATOM	562	N	ASP	231	-4.364	3.719	15.922	1.00	12.71
ATOM	563	CA	ASP	231	-4.951	3.496	14.603	1.00	12.71
ATOM	564	CB	ASP	231	-4.529	4.596	13.624	1.00	27.08
ATOM	565	CG	ASP	231	-5.053	5.967	14.020	1.00	27.08
ATOM	566	OD1	ASP	231	-6.144	6.047			



ATOM	567	OD2	ASP	231	-4.370	6.969	13.723	1.00	27.08
ATOM	568	C	ASP	231	-4.570	2.132	14.049	1.00	12.71
ATOM	569	O	ASP	231	-5.413	1.436	13.483	1.00	27.08
ATOM	570	N	PHE	232	-3.305	1.755	14.215	1.00	14.33
ATOM	571	CA	PHE	232	-2.823	0.461	13.748	1.00	14.33
ATOM	572	CB	PHE	232	-1.351	0.257	14.134	1.00	16.35
ATOM	573	CG	PHE	232	-0.911	-1.184	14.097	1.00	16.35
ATOM	574	CD1	PHE	232	-0.789	-1.862	12.887	1.00	16.35
ATOM	575	CD2	PHE	232	-0.661	-1.879	15.280	1.00	16.35
ATOM	576	CE1	PHE	232	-0.430	-3.208	12.851	1.00	16.35
ATOM	577	CE2	PHE	232	-0.302	-3.224	15.255	1.00	16.35
ATOM	578	CZ	PHE	232	-0.187	-3.890	14.038	1.00	16.35
ATOM	579	C	PHE	232	-3.670	-0.642	14.368	1.00	14.33
ATOM	580	O	PHE	232	-4.226	-1.482	13.661	1.00	16.35
ATOM	581	N	ALA	233	-3.769	-0.619	15.695	1.00	15.30
ATOM	582	CA	ALA	233	-4.537	-1.607	16.444	1.00	15.30
ATOM	583	CB	ALA	233	-4.413	-1.335	17.938	1.00	12.88
ATOM	584	C	ALA	233	-6.005	-1.609	16.030	1.00	15.30
ATOM	585	O	ALA	233	-6.627	-2.663	15.902	1.00	12.88
ATOM	586	N	LYS	234	-6.542	-0.419	15.795	1.00	25.69
ATOM	587	CA	LYS	234	-7.933	-0.256	15.401	1.00	25.69
ATOM	588	CB	LYS	234	-8.270	1.234	15.318	1.00	45.91
ATOM	589	CG	LYS	234	-9.574	1.595	15.979	1.00	45.91
ATOM	590	CD	LYS	234	-9.535	1.268	17.463	1.00	45.91
ATOM	591	CE	LYS	234	-10.938	1.047	18.006	1.00	45.91
ATOM	592	NZ	LYS	234	-11.605	-0.106	17.327	1.00	45.91
ATOM	593	C	LYS	234	-8.240	-0.931	14.067	1.00	25.69
ATOM	594	O	LYS	234	-9.368	-1.368	13.827	1.00	45.91
ATOM	595	N	LYS	235	-7.234	-1.019	13.204	1.00	17.44
ATOM	596	CA	LYS	235	-7.406	-1.627	11.892	1.00	17.44
ATOM	597	CB	LYS	235	-6.459	-0.975	10.884	1.00	26.26
ATOM	598	CG	LYS	235	-6.757	0.499	10.669	1.00	26.26
ATOM	599	CD	LYS	235	-5.785	1.141	9.706	1.00	26.26
ATOM	600	CE	LYS	235	-6.154	2.593	9.460	1.00	26.26
ATOM	601	NZ	LYS	235	-5.231	3.230	8.484	1.00	26.26
ATOM	602	C	LYS	235	-7.258	-3.146	11.875	1.00	17.44
ATOM	603	O	LYS	235	-7.365	-3.773	10.817	1.00	26.26
ATOM	604	N	LEU	236	-7.015	-3.738	13.040	1.00	21.99
ATOM	605	CA	LEU	236	-6.880	-5.187	13.144	1.00	21.99
ATOM	606	CB	LEU	236	-5.792	-5.564	14.154	1.00	25.38
ATOM	607	CG	LEU	236	-4.362	-5.127	13.818	1.00	25.38
ATOM	608	CD1	LEU	236	-3.415	-5.555	14.929	1.00	25.38
ATOM	609	CD2	LEU	236	-3.931	-5.725	12.491	1.00	25.38
ATOM	610	C	LEU	236	-8.219	-5.796	13.556	1.00	21.99
ATOM	611	O	LEU	236	-8.821	-5.386	14.553	1.00	25.38
ATOM	612	N	PRO	237	-8.682	-6.819	12.817	1.00	34.89
ATOM	613	CD	PRO	23					



ATOM	614	CA	PRO	237	-9.953	-7.513	13.071	1.00	34.89
ATOM	615	CB	PRO	237	-9.911	-8.687	12.084	1.00	42.99
ATOM	616	CG	PRO	237	-8.433	-8.887	11.816	1.00	42.99
ATOM	617	C	PRO	237	-10.184	-7.986	14.513	1.00	34.89
ATOM	618	O	PRO	237	-11.142	-7.563	15.159	1.00	42.99
ATOM	619	N <sup>-</sup>	MET	238	-9.301	-8.843	15.021	1.00	40.45
ATOM	620	CA	MET	238	-9.433	-9.364	16.382	1.00	40.45
ATOM	621	CB	MET	238	-8.360	-10.423	16.671	1.00	59.70
ATOM	622	CG	MET	238	-8.689	-11.839	16.195	1.00	59.70
ATOM	623	SD	MET	238	-8.013	-12.275	14.573	1.00	59.70
ATOM	624	CE	MET	238	-6.482	-13.074	15.032	1.00	59.70
ATOM	625	C	MET	238	-9.395	-8.305	17.486	1.00	40.45
ATOM	626	O	MET	238	-9.801	-8.574	18.617	1.00	59.70
ATOM	627	N	PHE	239	-8.928	-7.103	17.160	1.00	33.70
ATOM	628	CA	PHE	239	-8.829	-6.037	18.152	1.00	33.70
ATOM	629	CB	PHE	239	-7.651	-5.113	17.829	1.00	22.27
ATOM	630	CG	PHE	239	-7.386	-4.079	18.885	1.00	22.27
ATOM	631	CD1	PHE	239	-6.602	-4.385	19.990	1.00	22.27
ATOM	632	CD2	PHE	239	-7.926	-2.802	18.778	1.00	22.27
ATOM	633	CE1	PHE	239	-6.358	-3.436	20.974	1.00	22.27
ATOM	634	CE2	PHE	239	-7.688	-1.846	19.757	1.00	22.27
ATOM	635	CZ	PHE	239	-6.901	-2.163	20.857	1.00	22.27
ATOM	636	C	PHE	239	-10.103	-5.213	18.329	1.00	33.70
ATOM	637	O	PHE	239	-10.594	-5.059	19.446	1.00	22.27
ATOM	638	N	SER	240	-10.629	-4.679	17.232	1.00	23.42
ATOM	639	CA	SER	240	-11.837	-3.857	17.278	1.00	23.42
ATOM	640	CB	SER	240	-12.175	-3.352	15.884	1.00	26.21
ATOM	641	C	SER	240	-13.046	-4.562	17.899	1.00	23.42
ATOM	642	O	SER	240	-13.976	-3.909	18.369	1.00	26.21
ATOM	643	N	GLU	241	-13.028	-5.891	17.893	1.00	26.54
ATOM	644	CA	GLU	241	-14.116	-6.695	18.450	1.00	26.54
ATOM	645	CB	GLU	241	-14.007	-8.139	17.957	1.00	67.32
ATOM	646	CG	GLU	241	-14.241	-8.322	16.467	1.00	67.32
ATOM	647	CD	GLU	241	-13.979	-9.748	16.001	1.00	67.32
ATOM	648	OE1	GLU	241	-14.161	-10.691	16.803	1.00	67.32
ATOM	649	OE2	GLU	241	-13.584	-9.924	14.828	1.00	67.32
ATOM	650	C	GLU	241	-14.137	-6.706	19.975	1.00	26.54
ATOM	651	O	GLU	241	-15.182	-6.924	20.589	1.00	67.32
ATOM	652	N	LEU	242	-12.972	-6.506	20.579	1.00	26.16
ATOM	653	CA	LEU	242	-12.835	-6.514	22.030	1.00	26.16
ATOM	654	CB	LEU	242	-11.352	-6.473	22.412	1.00	19.79
ATOM	655	CG	LEU	242	-10.461	-7.627	21.956	1.00	19.79
ATOM	656	CD1	LEU	242	-9.014	-7.309	22.264	1.00	19.79
ATOM	657	CD2	LEU	242	-10.888	-8.912	22.640	1.00	19.79
ATOM	658	C	LEU	242	-13.547	-5.351	22.711	1.00	26.16
ATOM	659	O	LEU	242	-13.738	-4.290	22.115	1.00	19.79

ATOM	661	CD	PRO	243	-13.996	-6.785	24.764	1.00	19.17
ATOM	662	CA	PRO	243	-14.657	-4.454	24.671	1.00	17.98
ATOM	663	CB	PRO	243	-15.095	-5.105	25.988	1.00	19.17
ATOM	664	CG	PRO	243	-14.155	-6.263	26.161	1.00	19.17
ATOM	665	C	PRO	243	-13.652	-3.323	24.898	1.00	17.98
ATOM	666	O <sup>-</sup>	PRO	243	-12.458	-3.572	25.081	1.00	19.17
ATOM	667	N	CYS	244	-14.142	-2.088	24.880	1.00	20.08
ATOM	668	CA	CYS	244	-13.310	-0.900	25.059	1.00	20.08
ATOM	669	CB	CYS	244	-14.194	0.329	25.278	1.00	61.80
ATOM	670	SG	CYS	244	-13.674	1.784	24.340	1.00	61.80
ATOM	671	C	CYS	244	-12.286	-1.017	26.189	1.00	20.08
ATOM	672	O	CYS	244	-11.141	-0.590	26.040	1.00	61.80
ATOM	673	N	GLU	245	-12.691	-1.630	27.299	1.00	21.05
ATOM	674	CA	GLU	245	-11.814	-1.811	28.454	1.00	21.05
ATOM	675	CB	GLU	245	-12.541	-2.560	29.578	1.00	40.41
ATOM	676	CG	GLU	245	-13.510	-1.705	30.393	1.00	40.41
ATOM	677	CD	GLU	245	-14.953	-1.773	29.910	1.00	40.41
ATOM	678	OE1	GLU	245	-15.854	-1.761	30.775	1.00	40.41
ATOM	679	OE2	GLU	245	-15.197	-1.824	28.683	1.00	40.41
ATOM	680	C	GLU	245	-10.541	-2.558	28.084	1.00	21.05
ATOM	681	O	GLU	245	-9.439	-2.138	28.440	1.00	40.41
ATOM	682	N	ASP	246	-10.698	-3.654	27.351	1.00	17.22
ATOM	683	CA	ASP	246	-9.564	-4.463	26.924	1.00	17.22
ATOM	684	CB	ASP	246	-10.044	-5.774	26.303	1.00	30.41
ATOM	685	CG	ASP	246	-10.634	-6.727	27.327	1.00	30.41
ATOM	686	OD1	ASP	246	-10.755	-6.349	28.512	1.00	30.41
ATOM	687	OD2	ASP	246	-10.975	-7.864	26.946	1.00	30.41
ATOM	688	C	ASP	246	-8.693	-3.705	25.936	1.00	17.22
ATOM	689	O	ASP	246	-7.467	-3.713	26.050	1.00	30.41
ATOM	690	N	GLN	247	-9.332	-3.045	24.973	1.00	17.12
ATOM	691	CA	GLN	247	-8.615	-2.272	23.966	1.00	17.12
ATOM	692	CB	GLN	247	-9.594	-1.494	23.088	1.00	16.72
ATOM	693	CG	GLN	247	-10.504	-2.365	22.242	1.00	16.72
ATOM	694	CD	GLN	247	-11.352	-1.553	21.290	1.00	16.72
ATOM	695	OE1	GLN	247	-10.925	-0.515	20.790	1.00	16.72
ATOM	696	NE2	GLN	247	-12.560	-2.018	21.033	1.00	16.72
ATOM	697	C	GLN	247	-7.650	-1.303	24.637	1.00	17.12
ATOM	698	O	GLN	247	-6.476	-1.228	24.273	1.00	16.72
ATOM	699	N	ILE	248	-8.152	-0.591	25.640	1.00	19.19
ATOM	700	CA	ILE	248	-7.358	0.377	26.387	1.00	19.19
ATOM	701	CB	ILE	248	-8.238	1.137	27.410	1.00	24.32
ATOM	702	CG2	ILE	248	-7.385	2.055	28.282	1.00	24.32
ATOM	703	CG1	ILE	248	-9.312	1.942	26.668	1.00	24.32
ATOM	704	CD1	ILE	248	-10.327	2.618	27.573	1.00	24.32
ATOM	705	C	ILE	248	-6.180	-0.297	27.093	1.00	19.19
ATOM	706	O	ILE	248	-5.035	0.131	26.943	1.00	24.32

ATOM	708	CA	ILE	249	-5.409	-2.090	28.547	1.00	12.09
ATOM	709	CB	ILE	249	-5.996	-3.295	29.322	1.00	30.01
ATOM	710	CG2	ILE	249	-4.884	-4.168	29.885	1.00	30.01
ATOM	711	CG1	ILE	249	-6.899	-2.794	30.451	1.00	30.01
ATOM	712	CD1	ILE	249	-7.598	-3.893	31.215	1.00	30.01
ATOM	713	C <sup>+</sup>	ILE	249	-4.299	-2.561	27.602	1.00	12.09
ATOM	714	O	ILE	249	-3.115	-2.339	27.866	1.00	30.01
ATOM	715	N	LEU	250	-4.691	-3.168	26.486	1.00	20.87
ATOM	716	CA	LEU	250	-3.740	-3.669	25.498	1.00	20.87
ATOM	717	CB	LEU	250	-4.474	-4.410	24.376	1.00	15.15
ATOM	718	CG	LEU	250	-5.252	-5.669	24.761	1.00	15.15
ATOM	719	CD1	LEU	250	-5.907	-6.256	23.533	1.00	15.15
ATOM	720	CD2	LEU	250	-4.325	-6.686	25.400	1.00	15.15
ATOM	721	C	LEU	250	-2.900	-2.548	24.902	1.00	20.87
ATOM	722	O	LEU	250	-1.680	-2.667	24.792	1.00	15.15
ATOM	723	N	LEU	251	-3.559	-1.455	24.532	1.00	9.31
ATOM	724	CA	LEU	251	-2.887	-0.301	23.945	1.00	9.31
ATOM	725	CB	LEU	251	-3.920	0.760	23.553	1.00	19.90
ATOM	726	CG	LEU	251	-4.075	1.127	22.073	1.00	19.90
ATOM	727	CD1	LEU	251	-3.281	0.190	21.180	1.00	19.90
ATOM	728	CD2	LEU	251	-5.550	1.113	21.699	1.00	19.90
ATOM	729	C	LEU	251	-1.851	0.307	24.887	1.00	9.31
ATOM	730	O	LEU	251	-0.699	0.521	24.507	1.00	19.90
ATOM	731	N	LYS	252	-2.253	0.545	26.127	1.00	18.83
ATOM	732	CA	LYS	252	-1.362	1.132	27.114	1.00	18.83
ATOM	733	CB	LYS	252	-2.138	1.455	28.395	1.00	42.69
ATOM	734	CG	LYS	252	-3.395	2.274	28.130	1.00	42.69
ATOM	735	CD	LYS	252	-3.588	3.412	29.115	1.00	42.69
ATOM	736	CE	LYS	252	-3.998	2.934	30.493	1.00	42.69
ATOM	737	NZ	LYS	252	-4.300	4.109	31.361	1.00	42.69
ATOM	738	C	LYS	252	-0.171	0.222	27.408	1.00	18.83
ATOM	739	O	LYS	252	0.942	0.700	27.646	1.00	42.69
ATOM	740	N	GLY	253	-0.392	-1.086	27.328	1.00	16.16
ATOM	741	CA	GLY	253	0.676	-2.031	27.595	1.00	16.16
ATOM	742	C	GLY	253	1.688	-2.232	26.479	1.00	16.16
ATOM	743	O	GLY	253	2.836	-2.587	26.747	1.00	34.57
ATOM	744	N	CYS	254	1.286	-1.999	25.233	1.00	21.81
ATOM	745	CA	CYS	254	2.194	-2.203	24.108	1.00	21.81
ATOM	746	CB	CYS	254	1.563	-3.151	23.093	1.00	23.60
ATOM	747	SG	CYS	254	0.211	-2.387	22.179	1.00	23.60
ATOM	748	C	CYS	254	2.616	-0.935	23.380	1.00	21.81
ATOM	749	O	CYS	254	3.499	-0.983	22.521	1.00	23.60
ATOM	750	N	CYS	255	2.004	0.193	23.724	1.00	14.98
ATOM	751	CA	CYS	255	2.309	1.461	23.066	1.00	14.98
ATOM	752	CB	CYS	255	1.611	2.616	23.781	1.00	24.32
ATOM	753	SG	CYS	255	1.602	4.153	22.841	1.00	24.32
ATOM	754	C	CYS						

ATOM	755	O	CYS	255	4.305	1.895	21.805	1.00	24.32
ATOM	756	N	MET	256	4.525	1.777	24.037	1.00	13.77
ATOM	757	CA	MET	256	5.959	2.056	24.003	1.00	13.77
ATOM	758	CB	MET	256	6.515	2.218	25.423	1.00	19.23
ATOM	759	CG	MET	256	7.988	2.607	25.477	1.00	19.23
ATOM	760	SD	MET	256	8.344	4.132	24.571	1.00	19.23
ATOM	761	CE	MET	256	10.127	4.254	24.782	1.00	19.23
ATOM	762	C	MET	256	6.734	0.978	23.246	1.00	13.77
ATOM	763	O	MET	256	7.672	1.284	22.516	1.00	19.23
ATOM	764	N	GLU	257	6.316	-0.275	23.400	1.00	12.57
ATOM	765	CA	GLU	257	6.971	-1.397	22.730	1.00	12.57
ATOM	766	CB	GLU	257	6.342	-2.716	23.182	1.00	31.54
ATOM	767	CG	GLU	257	6.497	-2.982	24.677	1.00	31.54
ATOM	768	CD	GLU	257	5.720	-4.196	25.167	1.00	31.54
ATOM	769	OE1	GLU	257	5.220	-4.983	24.334	1.00	31.54
ATOM	770	OE2	GLU	257	5.607	-4.361	26.400	1.00	31.54
ATOM	771	C	GLU	257	6.889	-1.254	21.211	1.00	12.57
ATOM	772	O	GLU	257	7.881	-1.452	20.505	1.00	31.54
ATOM	773	N	ILE	258	5.712	-0.881	20.717	1.00	17.89
ATOM	774	CA	ILE	258	5.508	-0.692	19.288	1.00	17.89
ATOM	775	CB	ILE	258	4.001	-0.555	18.946	1.00	15.57
ATOM	776	CG2	ILE	258	3.813	-0.129	17.493	1.00	15.57
ATOM	777	CG1	ILE	258	3.288	-1.886	19.211	1.00	15.57
ATOM	778	CD1	ILE	258	1.798	-1.872	18.922	1.00	15.57
ATOM	779	C	ILE	258	6.289	0.535	18.811	1.00	17.89
ATOM	780	O	ILE	258	7.000	0.468	17.805	1.00	15.57
ATOM	781	N	MET	259	6.196	1.636	19.556	1.00	11.23
ATOM	782	CA	MET	259	6.907	2.861	19.201	1.00	11.23
ATOM	783	CB	MET	259	6.568	3.995	20.175	1.00	22.19
ATOM	784	CG	MET	259	5.112	4.439	20.117	1.00	22.19
ATOM	785	SD	MET	259	4.828	6.033	20.915	1.00	22.19
ATOM	786	CE	MET	259	5.038	5.606	22.621	1.00	22.19
ATOM	787	C	MET	259	8.415	2.637	19.131	1.00	11.23
ATOM	788	O	MET	259	9.060	3.008	18.145	1.00	22.19
ATOM	789	N	SER	260	8.974	1.994	20.153	1.00	8.59
ATOM	790	CA	SER	260	10.408	1.706	20.195	1.00	8.59
ATOM	791	CB	SER	260	10.763	0.939	21.472	1.00	23.39
ATOM	792	OG	SER	260	10.430	1.685	22.623	1.00	23.39
ATOM	793	C	SER	260	10.793	0.864	18.977	1.00	8.59
ATOM	794	O	SER	260	11.824	1.100	18.350	1.00	23.39
ATOM	795	N	LEU	261	9.952	-0.111	18.644	1.00	13.26
ATOM	796	CA	LEU	261	10.194	-0.992	17.507	1.00	13.26
ATOM	797	CB	LEU	261	9.076	-2.035	17.401	1.00	14.32
ATOM	798	CG	LEU	261	9.019	-2.894	16.134	1.00	14.32
ATOM	799	CD1	LEU	261	10.278	-3.733	15.999	1.00	14.32
ATOM	800	CD2	LEU	261	7.785	-3.772	16.174	1.00	14.32
ATOM	801	C	LEU	261					



ATOM	802	O	LEU	261	11.213	-0.313	15.432	1.00	14.32
ATOM	803	N	ARG	262	9.330	0.744	16.043	1.00	10.57
ATOM	804	CA	ARG	262	9.278	1.598	14.861	1.00	10.57
ATOM	805	CB	ARG	262	8.018	2.454	14.917	1.00	16.08
ATOM	806	CG	ARG	262	6.755	1.647	14.728	1.00	16.08
ATOM	807	CD	ARG	262	5.540	2.525	14.614	1.00	16.08
ATOM	808	NE	ARG	262	4.418	1.765	14.076	1.00	16.08
ATOM	809	CZ	ARG	262	3.260	2.289	13.689	1.00	16.08
ATOM	810	NH1	ARG	262	3.050	3.596	13.780	1.00	16.08
ATOM	811	NH2	ARG	262	2.322	1.497	13.183	1.00	16.08
ATOM	812	C	ARG	262	10.530	2.471	14.704	1.00	10.57
ATOM	813	O	ARG	262	11.038	2.649	13.589	1.00	16.08
ATOM	814	N	ALA	263	11.016	3.014	15.820	1.00	13.37
ATOM	815	CA	ALA	263	12.221	3.842	15.831	1.00	13.37
ATOM	816	CB	ALA	263	12.363	4.516	17.172	1.00	17.12
ATOM	817	C	ALA	263	13.443	2.964	15.561	1.00	13.37
ATOM	818	O	ALA	263	14.313	3.316	14.762	1.00	17.12
ATOM	819	N	ALA	264	13.474	1.802	16.207	1.00	16.55
ATOM	820	CA	ALA	264	14.574	0.855	16.072	1.00	16.55
ATOM	821	CB	ALA	264	14.375	-0.327	17.019	1.00	24.62
ATOM	822	C	ALA	264	14.770	0.364	14.642	1.00	16.55
ATOM	823	O	ALA	264	15.904	0.244	14.169	1.00	24.62
ATOM	824	N	VAL	265	13.670	0.073	13.955	1.00	22.25
ATOM	825	CA	VAL	265	13.754	-0.401	12.583	1.00	22.25
ATOM	826	CB	VAL	265	12.428	-1.038	12.086	1.00	25.31
ATOM	827	CG1	VAL	265	12.079	-2.239	12.936	1.00	25.31
ATOM	828	CG2	VAL	265	11.302	-0.030	12.091	1.00	25.31
ATOM	829	C	VAL	265	14.208	0.707	11.639	1.00	22.25
ATOM	830	O	VAL	265	14.615	0.434	10.513	1.00	25.31
ATOM	831	N	ARG	266	14.124	1.955	12.092	1.00	26.45
ATOM	832	CA	ARG	266	14.567	3.086	11.283	1.00	26.45
ATOM	833	CB	ARG	266	13.596	4.261	11.399	1.00	38.04
ATOM	834	CG	ARG	266	12.232	4.019	10.807	1.00	38.04
ATOM	835	CD	ARG	266	11.503	5.339	10.651	1.00	38.04
ATOM	836	NE	ARG	266	10.074	5.216	10.925	1.00	38.04
ATOM	837	CZ	ARG	266	9.504	5.551	12.079	1.00	38.04
ATOM	838	NH1	ARG	266	10.237	6.038	13.075	1.00	38.04
ATOM	839	NH2	ARG	266	8.196	5.411	12.240	1.00	38.04
ATOM	840	C	ARG	266	15.957	3.531	11.729	1.00	26.45
ATOM	841	O	ARG	266	16.296	4.717	11.660	1.00	38.04
ATOM	842	N	TYR	267	16.733	2.590	12.251	1.00	24.87
ATOM	843	CA	TYR	267	18.083	2.888	12.700	1.00	24.87
ATOM	844	CB	TYR	267	18.592	1.788	13.639	1.00	25.84
ATOM	845	CG	TYR	267	20.073	1.865	13.931	1.00	25.84
ATOM	846	CD1	TYR	267	20.579	2.789	14.844	1.00	25.84
ATOM	847	CE1	TYR	267	21.940	2.865	15.103	1.00	25.84
ATOM	848								



ATOM	849	CE2 TYR	267	22.331	1.085	13.536	1.00	25.84
ATOM	850	CZ TYR	267	22.810	2.011	14.444	1.00	25.84
ATOM	851	OH TYR	267	24.162	2.078	14.683	1.00	25.84
ATOM	852	C TYR	267	18.999	3.009	11.488	1.00	24.87
ATOM	853	O TYR	267	19.019	2.130	10.625	1.00	25.84
ATOM	854	N <sup>+</sup> ASP	268	19.751	4.102	11.423	1.00	28.13
ATOM	855	CA ASP	268	20.666	4.320	10.313	1.00	28.13
ATOM	856	CB ASP	268	20.524	5.744	9.773	1.00	51.63
ATOM	857	CG ASP	268	21.339	5.973	8.517	1.00	51.63
ATOM	858	OD1 ASP	268	21.060	5.305	7.498	1.00	51.63
ATOM	859	OD2 ASP	268	22.262	6.814	8.547	1.00	51.63
ATOM	860	C ASP	268	22.105	4.068	10.749	1.00	28.13
ATOM	861	O ASP	268	22.683	4.854	11.500	1.00	51.63
ATOM	862	N PRO	269	22.707	2.964	10.276	1.00	37.07
ATOM	863	CD PRO	269	22.103	1.938	9.410	1.00	39.18
ATOM	864	CA PRO	269	24.086	2.612	10.623	1.00	37.07
ATOM	865	CB PRO	269	24.319	1.324	9.832	1.00	39.18
ATOM	866	CG PRO	269	22.950	0.735	9.706	1.00	39.18
ATOM	867	C PRO	269	25.079	3.698	10.216	1.00	37.07
ATOM	868	O PRO	269	26.003	4.006	10.964	1.00	39.18
ATOM	869	N ALA	270	24.855	4.295	9.047	1.00	46.88
ATOM	870	CA ALA	270	25.730	5.340	8.519	1.00	46.88
ATOM	871	CB ALA	270	25.177	5.873	7.198	1.00	41.71
ATOM	872	C ALA	270	25.974	6.493	9.492	1.00	46.88
ATOM	873	O ALA	270	27.121	6.844	9.763	1.00	41.71
ATOM	874	N SER	271	24.899	7.081	10.009	1.00	34.54
ATOM	875	CA SER	271	25.013	8.198	10.941	1.00	34.54
ATOM	876	CB SER	271	23.959	9.259	10.618	1.00	42.29
ATOM	877	OG SER	271	22.686	8.668	10.422	1.00	42.29
ATOM	878	C SER	271	24.910	7.793	12.408	1.00	34.54
ATOM	879	O SER	271	25.169	8.607	13.297	1.00	42.29
ATOM	880	N ASP	272	24.546	6.535	12.653	1.00	41.05
ATOM	881	CA ASP	272	24.388	6.005	14.007	1.00	41.05
ATOM	882	CB ASP	272	25.720	6.078	14.772	1.00	47.32
ATOM	883	CG ASP	272	25.653	5.428	16.147	1.00	47.32
ATOM	884	OD1 ASP	272	24.981	4.384	16.299	1.00	47.32
ATOM	885	OD2 ASP	272	26.284	5.967	17.081	1.00	47.32
ATOM	886	C ASP	272	23.279	6.777	14.730	1.00	41.05
ATOM	887	O ASP	272	23.444	7.233	15.866	1.00	47.32
ATOM	888	N THR	273	22.139	6.905	14.058	1.00	27.60
ATOM	889	CA THR	273	20.996	7.618	14.608	1.00	27.60
ATOM	890	CB THR	273	20.808	8.991	13.911	1.00	30.96
ATOM	891	OG1 THR	273	20.723	8.808	12.491	1.00	30.96
ATOM	892	CG2 THR	273	21.967	9.924	14.228	1.00	30.96
ATOM	893	C THR	273	19.701	6.829	14.442	1.00	27.60
ATOM	894	O THR	273	19.633	5.883	13.650	1.00	30.96
ATOM	895	N LEU	274	18.696	7.192	15.232	1.00	20.89

ATOM	896	CA	LEU	274	17.374	6.574	15.161	1.00	20.89
ATOM	897	CB	LEU	274	16.862	6.193	16.555	1.00	22.48
ATOM	898	CG	LEU	274	17.480	5.009	17.301	1.00	22.48
ATOM	899	CD1	LEU	274	16.798	4.866	18.650	1.00	22.48
ATOM	900	CD2	LEU	274	17.317	3.736	16.497	1.00	22.48
ATOM	901	C <sup>+</sup>	LEU	274	16.470	7.654	14.586	1.00	20.89
ATOM	902	O	LEU	274	16.753	8.842	14.744	1.00	22.48
ATOM	903	N	THR	275	15.393	7.258	13.922	1.00	27.89
ATOM	904	CA	THR	275	14.478	8.235	13.354	1.00	27.89
ATOM	905	CB	THR	275	14.325	8.045	11.832	1.00	37.64
ATOM	906	OG1	THR	275	15.622	7.983	11.228	1.00	37.64
ATOM	907	CG2	THR	275	13.570	9.215	11.222	1.00	37.64
ATOM	908	C	THR	275	13.120	8.135	14.032	1.00	27.89
ATOM	909	O	THR	275	12.493	7.081	14.019	1.00	37.64
ATOM	910	N	LEU	276	12.700	9.226	14.667	1.00	28.07
ATOM	911	CA	LEU	276	11.418	9.275	15.358	1.00	28.07
ATOM	912	CB	LEU	276	11.497	10.214	16.572	1.00	24.81
ATOM	913	CG	LEU	276	12.639	10.005	17.577	1.00	24.81
ATOM	914	CD1	LEU	276	12.450	10.929	18.769	1.00	24.81
ATOM	915	CD2	LEU	276	12.692	8.558	18.038	1.00	24.81
ATOM	916	C	LEU	276	10.339	9.761	14.395	1.00	28.07
ATOM	917	O	LEU	276	10.533	10.760	13.691	1.00	24.81
ATOM	918	N	SER	277	9.232	9.027	14.331	1.00	29.24
ATOM	919	CA	SER	277	8.106	9.357	13.458	1.00	29.24
ATOM	920	CB	SER	277	7.369	10.594	13.985	1.00	30.56
ATOM	921	OG	SER	277	6.845	10.358	15.283	1.00	30.56
ATOM	922	C	SER	277	8.533	9.569	12.005	1.00	29.24
ATOM	923	O	SER	277	7.902	10.326	11.263	1.00	30.56
ATOM	924	N	GLY	278	9.619	8.908	11.618	1.00	34.41
ATOM	925	CA	GLY	278	10.135	9.024	10.263	1.00	34.41
ATOM	926	C	GLY	278	10.472	10.442	9.830	1.00	34.41
ATOM	927	O	GLY	278	10.516	10.725	8.631	1.00	44.04
ATOM	928	N	GLU	279	10.733	11.326	10.791	1.00	37.82
ATOM	929	CA	GLU	279	11.056	12.717	10.479	1.00	37.82
ATOM	930	CB	GLU	279	9.808	13.600	10.612	1.00	70.24
ATOM	931	CG	GLU	279	9.202	13.631	12.014	1.00	70.24
ATOM	932	CD	GLU	279	8.028	14.593	12.141	1.00	70.24
ATOM	933	OE1	GLU	279	8.028	15.406	13.093	1.00	70.24
ATOM	934	OE2	GLU	279	7.103	14.535	11.301	1.00	70.24
ATOM	935	C	GLU	279	12.192	13.321	11.300	1.00	37.82
ATOM	936	O	GLU	279	12.857	14.248	10.841	1.00	70.24
ATOM	937	N	MET	280	12.424	12.811	12.505	1.00	33.77
ATOM	938	CA	MET	280	13.482	13.360	13.344	1.00	33.77
ATOM	939	CB	MET	280	12.903	13.848	14.674	1.00	33.89
ATOM	940	CG	MET	280	13.898	14.595	15.545	1.00	33.89
ATOM	941	SD	MET	280	13.350	14.740			

ATOM	943	C	MET	280	14.620	12.383	13.613	1.00	33.77
ATOM	944	O	MET	280	14.432	11.366	14.282	1.00	33.89
ATOM	945	N	ALA	281	15.797	12.690	13.080	1.00	30.24
ATOM	946	CA	ALA	281	16.972	11.852	13.287	1.00	30.24
ATOM	947	CB	ALA	281	17.937	11.998	12.120	1.00	25.10
ATOM	948	C <sup>-</sup>	ALA	281	17.631	12.309	14.587	1.00	30.24
ATOM	949	O	ALA	281	18.008	13.477	14.718	1.00	25.10
ATOM	950	N	VAL	282	17.743	11.401	15.551	1.00	32.12
ATOM	951	CA	VAL	282	18.339	11.726	16.844	1.00	32.12
ATOM	952	CB	VAL	282	17.303	11.606	17.991	1.00	37.75
ATOM	953	CG1	VAL	282	16.184	12.615	17.799	1.00	37.75
ATOM	954	CG2	VAL	282	16.739	10.193	18.055	1.00	37.75
ATOM	955	C	VAL	282	19.543	10.852	17.181	1.00	32.12
ATOM	956	O	VAL	282	19.614	9.690	16.778	1.00	37.75
ATOM	957	N	LYS	283	20.491	11.428	17.913	1.00	26.82
ATOM	958	CA	LYS	283	21.700	10.722	18.328	1.00	26.82
ATOM	959	CB	LYS	283	22.894	11.679	18.342	1.00	57.25
ATOM	960	CG	LYS	283	23.258	12.245	16.979	1.00	57.25
ATOM	961	CD	LYS	283	24.282	13.361	17.105	1.00	57.25
ATOM	962	CE	LYS	283	24.752	13.836	15.741	1.00	57.25
ATOM	963	NZ	LYS	283	25.518	12.772	15.033	1.00	57.25
ATOM	964	C	LYS	283	21.509	10.120	19.717	1.00	26.82
ATOM	965	O	LYS	283	20.648	10.566	20.477	1.00	57.25
ATOM	966	N	ARG	284	22.351	9.146	20.058	1.00	26.41
ATOM	967	CA	ARG	284	22.297	8.457	21.351	1.00	26.41
ATOM	968	CB	ARG	284	23.527	7.566	21.528	1.00	41.02
ATOM	969	CG	ARG	284	23.715	6.539	20.440	1.00	41.02
ATOM	970	CD	ARG	284	25.016	5.794	20.616	1.00	41.02
ATOM	971	NE	ARG	284	25.145	4.730	19.630	1.00	41.02
ATOM	972	CZ	ARG	284	24.759	3.475	19.831	1.00	41.02
ATOM	973	NH1	ARG	284	24.221	3.117	20.990	1.00	41.02
ATOM	974	NH2	ARG	284	24.886	2.584	18.859	1.00	41.02
ATOM	975	C	ARG	284	22.200	9.399	22.543	1.00	26.41
ATOM	976	O	ARG	284	21.296	9.278	23.370	1.00	41.02
ATOM	977	N	GLU	285	23.152	10.321	22.634	1.00	33.23
ATOM	978	CA	GLU	285	23.201	11.292	23.721	1.00	33.23
ATOM	979	CB	GLU	285	24.366	12.258	23.492	1.00	69.82
ATOM	980	CG	GLU	285	24.485	13.359	24.533	1.00	69.82
ATOM	981	CD	GLU	285	25.079	14.636	23.964	1.00	69.82
ATOM	982	OE1	GLU	285	26.309	14.826	24.070	1.00	69.82
ATOM	983	OE2	GLU	285	24.309	15.453	23.409	1.00	69.82
ATOM	984	C	GLU	285	21.898	12.082	23.823	1.00	33.23
ATOM	985	O	GLU	285	21.336	12.239	24.907	1.00	69.82
ATOM	986	N	GLN	286	21.414	12.551	22.677	1.00	28.07
ATOM	987	CA	GLN	286	20.194	13.346	22.614	1.00	28.07
ATOM	988	CB	GLN	286	19.9				

ATOM	990	CD	GLN	286	20.808	15.154	19.202	1.00	41.05
ATOM	991	OE1	GLN	286	20.783	14.322	18.293	1.00	41.05
ATOM	992	NE2	GLN	286	20.635	16.452	18.990	1.00	41.05
ATOM	993	C	GLN	286	18.955	12.642	23.162	1.00	28.07
ATOM	994	O	GLN	286	18.281	13.174	24.048	1.00	41.05
ATOM	995	N <sup>+</sup>	LEU	287	18.663	11.447	22.658	1.00	30.11
ATOM	996	CA	LEU	287	17.492	10.705	23.116	1.00	30.11
ATOM	997	CB	LEU	287	17.232	9.489	22.219	1.00	21.70
ATOM	998	CG	LEU	287	15.859	8.821	22.357	1.00	21.70
ATOM	999	CD1	LEU	287	14.748	9.818	22.061	1.00	21.70
ATOM	1000	CD2	LEU	287	15.763	7.628	21.421	1.00	21.70
ATOM	1001	C	LEU	287	17.641	10.277	24.577	1.00	30.11
ATOM	1002	O	LEU	287	16.655	10.212	25.320	1.00	21.70
ATOM	1003	N	LYS	288	18.878	10.015	24.992	1.00	20.72
ATOM	1004	CA	LYS	288	19.156	9.611	26.365	1.00	20.72
ATOM	1005	CB	LYS	288	20.626	9.213	26.514	1.00	43.14
ATOM	1006	CG	LYS	288	20.991	8.721	27.903	1.00	43.14
ATOM	1007	CD	LYS	288	22.374	8.102	27.931	1.00	43.14
ATOM	1008	CE	LYS	288	22.615	7.379	29.250	1.00	43.14
ATOM	1009	NZ	LYS	288	23.866	6.568	29.224	1.00	43.14
ATOM	1010	C	LYS	288	18.819	10.742	27.331	1.00	20.72
ATOM	1011	O	LYS	288	18.027	10.566	28.261	1.00	43.14
ATOM	1012	N	ASN	289	19.380	11.917	27.067	1.00	33.64
ATOM	1013	CA	ASN	289	19.156	13.090	27.906	1.00	33.64
ATOM	1014	CB	ASN	289	20.190	14.173	27.590	1.00	35.61
ATOM	1015	CG	ASN	289	21.607	13.730	27.898	1.00	35.61
ATOM	1016	OD1	ASN	289	21.835	12.920	28.797	1.00	35.61
ATOM	1017	ND2	ASN	289	22.566	14.253	27.149	1.00	35.61
ATOM	1018	C	ASN	289	17.747	13.654	27.757	1.00	33.64
ATOM	1019	O	ASN	289	17.276	14.399	28.616	1.00	35.61
ATOM	1020	N	GLY	290	17.072	13.287	26.672	1.00	22.05
ATOM	1021	CA	GLY	290	15.722	13.767	26.435	1.00	22.05
ATOM	1022	C	GLY	290	14.688	13.247	27.416	1.00	22.05
ATOM	1023	O	GLY	290	13.550	13.710	27.420	1.00	29.95
ATOM	1024	N	GLY	291	15.072	12.276	28.239	1.00	24.91
ATOM	1025	CA	GLY	291	14.142	11.732	29.211	1.00	24.91
ATOM	1026	C	GLY	291	14.093	10.217	29.248	1.00	24.91
ATOM	1027	O	GLY	291	13.536	9.640	30.179	1.00	29.39
ATOM	1028	N	LEU	292	14.676	9.567	28.246	1.00	30.21
ATOM	1029	CA	LEU	292	14.675	8.110	28.189	1.00	30.21
ATOM	1030	CB	LEU	292	14.732	7.626	26.734	1.00	21.45
ATOM	1031	CG	LEU	292	13.439	7.795	25.928	1.00	21.45
ATOM	1032	CD1	LEU	292	13.612	7.225	24.542	1.00	21.45
ATOM	1033	CD2	LEU	292	12.296	7.087	26.630	1.00	21.45
ATOM	1034	C	LEU	292	15.785	7.461	29.013	1.00	30.21
ATOM	1035	O	LEU	292	15.645	6.324	29.473	1.00	21.45
ATOM	1036	N	GLY	293	16.885	8.180	29.205	1.00	16.29



ATOM	1037	CA	GLY	293	17.992	7.638	29.970	1.00	16.29
ATOM	1038	C	GLY	293	18.534	6.374	29.332	1.00	16.29
ATOM	1039	O	GLY	293	18.763	6.334	28.122	1.00	25.88
ATOM	1040	N	VAL	294	18.689	5.322	30.130	1.00	33.05
ATOM	1041	CA	VAL	294	19.211	4.050	29.635	1.00	33.05
ATOM	1042	CB	VAL	294	19.530	3.069	30.788	1.00	30.11
ATOM	1043	CG1	VAL	294	20.718	3.577	31.582	1.00	30.11
ATOM	1044	CG2	VAL	294	18.315	2.887	31.697	1.00	30.11
ATOM	1045	C	VAL	294	18.302	3.361	28.617	1.00	33.05
ATOM	1046	O	VAL	294	18.768	2.545	27.817	1.00	30.11
ATOM	1047	N	VAL	295	17.014	3.699	28.635	1.00	18.14
ATOM	1048	CA	VAL	295	16.056	3.118	27.698	1.00	18.14
ATOM	1049	CB	VAL	295	14.638	3.698	27.902	1.00	28.34
ATOM	1050	CG1	VAL	295	13.668	3.099	26.893	1.00	28.34
ATOM	1051	CG2	VAL	295	14.159	3.431	29.317	1.00	28.34
ATOM	1052	C	VAL	295	16.521	3.415	26.275	1.00	18.14
ATOM	1053	O	VAL	295	16.395	2.577	25.383	1.00	28.34
ATOM	1054	N	SER	296	17.091	4.601	26.085	1.00	20.84
ATOM	1055	CA	SER	296	17.596	5.028	24.785	1.00	20.84
ATOM	1056	CB	SER	296	18.160	6.446	24.884	1.00	25.61
ATOM	1057	OG	SER	296	18.615	6.911	23.627	1.00	25.61
ATOM	1058	C	SER	296	18.687	4.074	24.307	1.00	20.84
ATOM	1059	O	SER	296	18.723	3.691	23.133	1.00	25.61
ATOM	1060	N	ASP	297	19.571	3.691	25.224	1.00	28.08
ATOM	1061	CA	ASP	297	20.660	2.777	24.904	1.00	28.08
ATOM	1062	CB	ASP	297	21.555	2.552	26.129	1.00	51.15
ATOM	1063	CG	ASP	297	22.207	3.835	26.629	1.00	51.15
ATOM	1064	OD1	ASP	297	22.508	4.725	25.804	1.00	51.15
ATOM	1065	OD2	ASP	297	22.425	3.948	27.855	1.00	51.15
ATOM	1066	C	ASP	297	20.079	1.450	24.434	1.00	28.08
ATOM	1067	O	ASP	297	20.549	0.869	23.456	1.00	51.15
ATOM	1068	N	ALA	298	19.024	1.006	25.111	1.00	26.12
ATOM	1069	CA	ALA	298	18.357	-0.245	24.778	1.00	26.12
ATOM	1070	CB	ALA	298	17.253	-0.530	25.787	1.00	18.80
ATOM	1071	C	ALA	298	17.790	-0.223	23.356	1.00	26.12
ATOM	1072	O	ALA	298	18.014	-1.154	22.575	1.00	18.80
ATOM	1073	N	ILE	299	17.078	0.848	23.013	1.00	17.42
ATOM	1074	CA	ILE	299	16.483	0.979	21.686	1.00	17.42
ATOM	1075	CB	ILE	299	15.559	2.211	21.597	1.00	16.69
ATOM	1076	CG2	ILE	299	14.845	2.238	20.253	1.00	16.69
ATOM	1077	CG1	ILE	299	14.515	2.149	22.712	1.00	16.69
ATOM	1078	CD1	ILE	299	13.713	3.406	22.872	1.00	16.69
ATOM	1079	C	ILE	299	17.563	1.042	20.609	1.00	17.42
ATOM	1080	O	ILE	299	17.416	0.443	19.542	1.00	16.69
ATOM	1081	N	PHE	300	18.652	1.752	20.889	1.00	14.46
ATOM	1082	CA	PHE	300	19.751	1.8			



ATOM	1084	CG	PHE	300	20.656	4.221	19.801	1.00	24.01
ATOM	1085	CD1	PHE	300	19.904	5.204	20.435	1.00	24.01
ATOM	1086	CD2	PHE	300	21.271	4.526	18.591	1.00	24.01
ATOM	1087	CE1	PHE	300	19.766	6.472	19.873	1.00	24.01
ATOM	1088	CE2	PHE	300	21.140	5.791	18.020	1.00	24.01
ATOM	1089	CZ	PHE	300	20.385	6.765	18.663	1.00	24.01
ATOM	1090	C	PHE	300	20.383	0.480	19.726	1.00	14.46
ATOM	1091	O	PHE	300	20.696	0.102	18.596	1.00	24.01
ATOM	1092	N	GLU	301	20.547	-0.270	20.813	1.00	21.61
ATOM	1093	CA	GLU	301	21.123	-1.609	20.744	1.00	21.61
ATOM	1094	CB	GLU	301	21.289	-2.192	22.143	1.00	23.89
ATOM	1095	C	GLU	301	20.211	-2.498	19.904	1.00	21.61
ATOM	1096	O	GLU	301	20.681	-3.251	19.043	1.00	23.89
ATOM	1097	N	LEU	302	18.906	-2.390	20.140	1.00	14.43
ATOM	1098	CA	LEU	302	17.922	-3.168	19.399	1.00	14.43
ATOM	1099	CB	LEU	302	16.512	-2.872	19.912	1.00	23.43
ATOM	1100	CG	LEU	302	15.350	-3.669	19.312	1.00	23.43
ATOM	1101	CD1	LEU	302	15.459	-5.140	19.688	1.00	23.43
ATOM	1102	CD2	LEU	302	14.035	-3.094	19.804	1.00	23.43
ATOM	1103	C	LEU	302	18.027	-2.812	17.917	1.00	14.43
ATOM	1104	O	LEU	302	18.089	-3.697	17.066	1.00	23.43
ATOM	1105	N	GLY	303	18.098	-1.515	17.625	1.00	15.17
ATOM	1106	CA	GLY	303	18.208	-1.056	16.251	1.00	15.17
ATOM	1107	C	GLY	303	19.411	-1.640	15.530	1.00	15.17
ATOM	1108	O	GLY	303	19.290	-2.137	14.406	1.00	27.67
ATOM	1109	N	LYS	304	20.570	-1.594	16.182	1.00	19.04
ATOM	1110	CA	LYS	304	21.802	-2.127	15.605	1.00	19.04
ATOM	1111	CB	LYS	304	22.979	-1.975	16.577	1.00	56.94
ATOM	1112	CG	LYS	304	23.496	-0.556	16.741	1.00	56.94
ATOM	1113	CD	LYS	304	24.811	-0.524	17.516	1.00	56.94
ATOM	1114	CE	LYS	304	24.634	-0.965	18.968	1.00	56.94
ATOM	1115	NZ	LYS	304	23.838	0.008	19.778	1.00	56.94
ATOM	1116	C	LYS	304	21.653	-3.596	15.229	1.00	19.04
ATOM	1117	O	LYS	304	21.974	-3.993	14.107	1.00	56.94
ATOM	1118	N	SER	305	21.146	-4.394	16.164	1.00	24.46
ATOM	1119	CA	SER	305	20.965	-5.822	15.932	1.00	24.46
ATOM	1120	CB	SER	305	20.610	-6.533	17.240	1.00	37.46
ATOM	1121	OG	SER	305	19.444	-5.984	17.827	1.00	37.46
ATOM	1122	C	SER	305	19.926	-6.128	14.853	1.00	24.46
ATOM	1123	O	SER	305	20.146	-6.996	14.006	1.00	37.46
ATOM	1124	N	LEU	306	18.819	-5.390	14.858	1.00	25.47
ATOM	1125	CA	LEU	306	17.753	-5.592	13.881	1.00	25.47
ATOM	1126	CB	LEU	306	16.525	-4.746	14.224	1.00	15.99
ATOM	1127	CG	LEU	306	15.700	-5.190	15.432	1.00	15.99
ATOM	1128	CD1	LEU	306	14.504	-4.271	15.600	1.00	15.99
ATOM	1129	CD2	LEU	306	15.244	-6.624	15.247	1.00	15.99
ATOM	1130	C	LEU	306	18.174	-5.330	12.439	1.00	25.47

ATOM	1131	O	LEU	306	17.596	-5.902	11.513	1.00	15.99
ATOM	1132	N	SER	307	19.182	-4.482	12.247	1.00	24.28
ATOM	1133	CA	SER	307	19.670	-4.160	10.907	1.00	24.28
ATOM	1134	CB	SER	307	20.910	-3.263	10.989	1.00	40.92
ATOM	1135	OG	SER	307	20.617	-2.028	11.622	1.00	40.92
ATOM	1136	C	SER	307	19.995	-5.422	10.107	1.00	24.28
ATOM	1137	O	SER	307	19.625	-5.535	8.936	1.00	40.92
ATOM	1138	N	ALA	308	20.644	-6.383	10.761	1.00	30.97
ATOM	1139	CA	ALA	308	21.027	-7.640	10.124	1.00	30.97
ATOM	1140	CB	ALA	308	22.004	-8.399	11.013	1.00	37.84
ATOM	1141	C	ALA	308	19.830	-8.528	9.779	1.00	30.97
ATOM	1142	O	ALA	308	19.897	-9.336	8.853	1.00	37.84
ATOM	1143	N	PHE	309	18.737	-8.372	10.520	1.00	22.78
ATOM	1144	CA	PHE	309	17.533	-9.166	10.292	1.00	22.78
ATOM	1145	CB	PHE	309	16.571	-9.037	11.477	1.00	30.14
ATOM	1146	CG	PHE	309	17.032	-9.751	12.716	1.00	30.14
ATOM	1147	CD1	PHE	309	16.299	-10.809	13.236	1.00	30.14
ATOM	1148	CD2	PHE	309	18.204	-9.372	13.359	1.00	30.14
ATOM	1149	CE1	PHE	309	16.725	-11.481	14.378	1.00	30.14
ATOM	1150	CE2	PHE	309	18.640	-10.038	14.503	1.00	30.14
ATOM	1151	CZ	PHE	309	17.896	-11.094	15.013	1.00	30.14
ATOM	1152	C	PHE	309	16.818	-8.813	8.990	1.00	22.78
ATOM	1153	O	PHE	309	16.068	-9.631	8.451	1.00	30.14
ATOM	1154	N	ASN	310	17.051	-7.598	8.496	1.00	35.30
ATOM	1155	CA	ASN	310	16.441	-7.109	7.255	1.00	35.30
ATOM	1156	CB	ASN	310	17.109	-7.760	6.037	1.00	28.28
ATOM	1157	C	ASN	310	14.929	-7.339	7.229	1.00	35.30
ATOM	1158	O	ASN	310	14.395	-7.970	6.312	1.00	28.28
ATOM	1159	N	LEU	311	14.249	-6.831	8.251	1.00	27.52
ATOM	1160	CA	LEU	311	12.803	-6.979	8.369	1.00	27.52
ATOM	1161	CB	LEU	311	12.351	-6.630	9.788	1.00	22.62
ATOM	1162	CG	LEU	311	12.950	-7.396	10.968	1.00	22.62
ATOM	1163	CD1	LEU	311	12.360	-6.864	12.268	1.00	22.62
ATOM	1164	CD2	LEU	311	12.672	-8.881	10.821	1.00	22.62
ATOM	1165	C	LEU	311	12.060	-6.085	7.382	1.00	27.52
ATOM	1166	O	LEU	311	12.519	-4.986	7.067	1.00	22.62
ATOM	1167	N	ASP	312	10.918	-6.563	6.892	1.00	16.74
ATOM	1168	CA	ASP	312	10.095	-5.789	5.968	1.00	16.74
ATOM	1169	CB	ASP	312	9.803	-6.578	4.673	1.00	16.35
ATOM	1170	CG	ASP	312	8.924	-7.814	4.888	1.00	16.35
ATOM	1171	OD1	ASP	312	8.591	-8.168	6.037	1.00	16.35
ATOM	1172	OD2	ASP	312	8.559	-8.446	3.876	1.00	16.35
ATOM	1173	C	ASP	312	8.808	-5.354	6.678	1.00	16.74
ATOM	1174	O	ASP	312	8.535	-5.798	7.797	1.00	16.35
ATOM	1175	N	ASP	313	8.007	-4.520	6.019	1.00	5.43
ATOM	1176	CA	ASP	313	6.758	-4.016	6.592	1.00	

ATOM	1178	CG ASP	313	6.670	-1.906	5.183	1.00	31.80
ATOM	1179	OD1 ASP	313	7.392	-1.340	6.033	1.00	31.80
ATOM	1180	OD2 ASP	313	6.493	-1.452	4.032	1.00	31.80
ATOM	1181	C ASP	313	5.849	-5.081	7.189	1.00	5.43
ATOM	1182	O ASP	313	5.216	-4.849	8.221	1.00	31.80
ATOM	1183	N THR	314	5.777	-6.238	6.543	1.00	12.98
ATOM	1184	CA THR	314	4.934	-7.327	7.022	1.00	12.98
ATOM	1185	CB THR	314	4.825	-8.441	5.968	1.00	18.90
ATOM	1186	OG1 THR	314	4.249	-7.904	4.769	1.00	18.90
ATOM	1187	CG2 THR	314	3.960	-9.578	6.477	1.00	18.90
ATOM	1188	C THR	314	5.426	-7.910	8.349	1.00	12.98
ATOM	1189	O THR	314	4.636	-8.124	9.268	1.00	18.90
ATOM	1190	N GLU	315	6.731	-8.135	8.457	1.00	9.13
ATOM	1191	CA GLU	315	7.316	-8.685	9.675	1.00	9.13
ATOM	1192	CB GLU	315	8.771	-9.078	9.427	1.00	11.49
ATOM	1193	CG GLU	315	8.870	-10.323	8.562	1.00	11.49
ATOM	1194	CD GLU	315	10.233	-10.544	7.945	1.00	11.49
ATOM	1195	OE1 GLU	315	10.964	-9.561	7.705	1.00	11.49
ATOM	1196	OE2 GLU	315	10.558	-11.715	7.669	1.00	11.49
ATOM	1197	C GLU	315	7.180	-7.720	10.847	1.00	9.13
ATOM	1198	O GLU	315	6.863	-8.131	11.967	1.00	11.49
ATOM	1199	N VAL	316	7.376	-6.433	10.575	1.00	9.46
ATOM	1200	CA VAL	316	7.240	-5.406	11.602	1.00	9.46
ATOM	1201	CB VAL	316	7.655	-4.015	11.063	1.00	7.95
ATOM	1202	CG1 VAL	316	7.434	-2.941	12.124	1.00	7.95
ATOM	1203	CG2 VAL	316	9.112	-4.037	10.625	1.00	7.95
ATOM	1204	C VAL	316	5.777	-5.365	12.051	1.00	9.46
ATOM	1205	O VAL	316	5.484	-5.300	13.247	1.00	7.95
ATOM	1206	N ALA	317	4.866	-5.438	11.083	1.00	5.52
ATOM	1207	CA ALA	317	3.434	-5.417	11.355	1.00	5.52
ATOM	1208	CB ALA	317	2.656	-5.415	10.054	1.00	10.98
ATOM	1209	C ALA	317	3.002	-6.595	12.225	1.00	5.52
ATOM	1210	O ALA	317	2.317	-6.412	13.230	1.00	10.98
ATOM	1211	N LEU	318	3.411	-7.799	11.838	1.00	8.62
ATOM	1212	CA LEU	318	3.067	-9.003	12.584	1.00	8.62
ATOM	1213	CB LEU	318	3.523	-10.249	11.825	1.00	10.49
ATOM	1214	CG LEU	318	2.770	-10.494	10.514	1.00	10.49
ATOM	1215	CD1 LEU	318	3.376	-11.664	9.769	1.00	10.49
ATOM	1216	CD2 LEU	318	1.297	-10.741	10.799	1.00	10.49
ATOM	1217	C LEU	318	3.674	-8.971	13.978	1.00	8.62
ATOM	1218	O LEU	318	3.047	-9.407	14.945	1.00	10.49
ATOM	1219	N LEU	319	4.885	-8.435	14.082	1.00	9.43
ATOM	1220	CA LEU	319	5.560	-8.325	15.366	1.00	9.43
ATOM	1221	CB LEU	319	6.975	-7.773	15.173	1.00	24.05
ATOM	1222	CG LEU	319	7.901	-7.680	16.389	1.00	24.05
ATOM	1223	CD1 LEU	319	7.889	-8.977	17.182	1.00	24.05
ATOM	1224	CD2 LEU	319	9.310	-7.356	15.922	1.00	24.05

ATOM	1225	C	LEU	319	4.731	-7.404	16.259	1.00	9.43
ATOM	1226	O	LEU	319	4.456	-7.731	17.416	1.00	24.05
ATOM	1227	N	GLN	320	4.287	-6.282	15.699	1.00	8.67
ATOM	1228	CA	GLN	320	3.467	-5.325	16.437	1.00	8.67
ATOM	1229	CB	GLN	320	3.151	-4.102	15.573	1.00	10.94
ATOM	1230	C $\bar{G}$	GLN	320	4.361	-3.256	15.218	1.00	10.94
ATOM	1231	CD	GLN	320	4.025	-2.045	14.359	1.00	10.94
ATOM	1232	OE1	GLN	320	4.889	-1.217	14.082	1.00	10.94
ATOM	1233	NE2	GLN	320	2.773	-1.940	13.924	1.00	10.94
ATOM	1234	C	GLN	320	2.169	-5.984	16.895	1.00	8.67
ATOM	1235	O	GLN	320	1.708	-5.751	18.013	1.00	10.94
ATOM	1236	N	ALA	321	1.586	-6.806	16.028	1.00	9.21
ATOM	1237	CA	ALA	321	0.349	-7.513	16.342	1.00	9.21
ATOM	1238	CB	ALA	321	-0.136	-8.283	15.129	1.00	12.83
ATOM	1239	C	ALA	321	0.558	-8.460	17.523	1.00	9.21
ATOM	1240	O	ALA	321	-0.315	-8.591	18.382	1.00	12.83
ATOM	1241	N	VAL	322	1.718	-9.111	17.566	1.00	9.10
ATOM	1242	CA	VAL	322	2.043	-10.030	18.651	1.00	9.10
ATOM	1243	CB	VAL	322	3.340	-10.827	18.352	1.00	15.92
ATOM	1244	CG1	VAL	322	3.783	-11.614	19.575	1.00	15.92
ATOM	1245	CG2	VAL	322	3.106	-11.780	17.194	1.00	15.92
ATOM	1246	C	VAL	322	2.192	-9.256	19.960	1.00	9.10
ATOM	1247	O	VAL	322	1.707	-9.691	21.003	1.00	15.92
ATOM	1248	N	LEU	323	2.856	-8.106	19.893	1.00	11.07
ATOM	1249	CA	LEU	323	3.062	-7.257	21.064	1.00	11.07
ATOM	1250	CB	LEU	323	3.959	-6.070	20.705	1.00	16.31
ATOM	1251	CG	LEU	323	5.377	-6.393	20.229	1.00	16.31
ATOM	1252	CD1	LEU	323	6.039	-5.149	19.669	1.00	16.31
ATOM	1253	CD2	LEU	323	6.187	-6.966	21.375	1.00	16.31
ATOM	1254	C	LEU	323	1.729	-6.742	21.595	1.00	11.07
ATOM	1255	O	LEU	323	1.523	-6.650	22.803	1.00	16.31
ATOM	1256	N	LEU	324	0.827	-6.413	20.677	1.00	13.48
ATOM	1257	CA	LEU	324	-0.494	-5.900	21.015	1.00	13.48
ATOM	1258	CB	LEU	324	-1.185	-5.383	19.752	1.00	15.92
ATOM	1259	CG	LEU	324	-2.607	-4.837	19.889	1.00	15.92
ATOM	1260	CD1	LEU	324	-2.602	-3.547	20.692	1.00	15.92
ATOM	1261	CD2	LEU	324	-3.182	-4.598	18.511	1.00	15.92
ATOM	1262	C	LEU	324	-1.393	-6.924	21.707	1.00	13.48
ATOM	1263	O	LEU	324	-1.896	-6.678	22.802	1.00	15.92
ATOM	1264	N	MET	325	-1.593	-8.074	21.072	1.00	11.47
ATOM	1265	CA	MET	325	-2.458	-9.111	21.631	1.00	11.47
ATOM	1266	CB	MET	325	-2.959	-10.043	20.520	1.00	22.90
ATOM	1267	CG	MET	325	-3.689	-9.347	19.375	1.00	22.90
ATOM	1268	SD	MET	325	-5.052	-8.287	19.908	1.00	22.90
ATOM	1269	CE	MET	325	-6.284	-9.475	20.353	1.00	22.90
ATOM	1270	C	MET	325	-1.814	-9.932	22.752	1	



ATOM	1272	N	SER	326	-1.193	-9.256	23.711	1.00	30.07
ATOM	1273	CA	SER	326	-0.543	-9.936	24.826	1.00	30.07
ATOM	1274	CB	SER	326	0.723	-9.175	25.239	1.00	32.79
ATOM	1275	OG	SER	326	1.283	-9.699	26.433	1.00	32.79
ATOM	1276	C	SER	326	-1.492	-10.061	26.014	1.00	30.07
ATOM	1277	O	SER	326	-2.343	-9.198	26.235	1.00	32.79
ATOM	1278	N	THR	327	-1.347	-11.143	26.773	1.00	29.08
ATOM	1279	CA	THR	327	-2.179	-11.368	27.948	1.00	29.08
ATOM	1280	CB	THR	327	-2.705	-12.817	27.998	1.00	36.96
ATOM	1281	OG1	THR	327	-1.612	-13.734	27.856	1.00	36.96
ATOM	1282	CG2	THR	327	-3.716	-13.055	26.890	1.00	36.96
ATOM	1283	C	THR	327	-1.426	-11.049	29.239	1.00	29.08
ATOM	1284	O	THR	327	-1.930	-11.295	30.333	1.00	36.96
ATOM	1285	N	ASP	328	-0.214	-10.513	29.111	1.00	38.93
ATOM	1286	CA	ASP	328	0.596	-10.152	30.273	1.00	38.93
ATOM	1287	CB	ASP	328	2.082	-10.089	29.899	1.00	85.70
ATOM	1288	CG	ASP	328	2.660	-11.451	29.556	1.00	85.70
ATOM	1289	OD1	ASP	328	3.388	-11.554	28.542	1.00	85.70
ATOM	1290	OD2	ASP	328	2.393	-12.418	30.303	1.00	85.70
ATOM	1291	C	ASP	328	0.148	-8.810	30.845	1.00	38.93
ATOM	1292	O	ASP	328	0.962	-7.911	31.061	1.00	85.70
ATOM	1293	N	ARG	329	-1.154	-8.673	31.070	1.00	28.95
ATOM	1294	CA	ARG	329	-1.716	-7.445	31.608	1.00	28.95
ATOM	1295	CB	ARG	329	-2.390	-6.612	30.509	1.00	38.88
ATOM	1296	CG	ARG	329	-1.449	-5.887	29.554	1.00	38.88
ATOM	1297	CD	ARG	329	-1.107	-6.739	28.347	1.00	38.88
ATOM	1298	NE	ARG	329	-0.322	-6.005	27.356	1.00	38.88
ATOM	1299	CZ	ARG	329	1.006	-5.936	27.351	1.00	38.88
ATOM	1300	NH1	ARG	329	1.713	-6.552	28.290	1.00	38.88
ATOM	1301	NH2	ARG	329	1.631	-5.270	26.391	1.00	38.88
ATOM	1302	C	ARG	329	-2.745	-7.790	32.672	1.00	28.95
ATOM	1303	O	ARG	329	-3.279	-8.898	32.696	1.00	38.88
ATOM	1304	N	SER	330	-3.029	-6.829	33.542	1.00	42.07
ATOM	1305	CA	SER	330	-3.999	-7.025	34.607	1.00	42.07
ATOM	1306	CB	SER	330	-3.488	-6.399	35.899	1.00	37.35
ATOM	1307	C	SER	330	-5.340	-6.413	34.220	1.00	42.07
ATOM	1308	O	SER	330	-5.386	-5.382	33.550	1.00	37.35
ATOM	1309	N	GLY	331	-6.424	-7.085	34.598	1.00	26.57
ATOM	1310	CA	GLY	331	-7.754	-6.572	34.318	1.00	26.57
ATOM	1311	C	GLY	331	-8.404	-6.915	32.991	1.00	26.57
ATOM	1312	O	GLY	331	-9.462	-6.371	32.671	1.00	30.06
ATOM	1313	N	LEU	332	-7.797	-7.807	32.214	1.00	31.47
ATOM	1314	CA	LEU	332	-8.374	-8.189	30.928	1.00	31.47
ATOM	1315	CB	LEU	332	-7.351	-8.933	30.065	1.00	23.83
ATOM	1316	CG	LEU	332	-6.261	-8.076	29.425	1.00	23.83
ATOM	1317	CD1	LEU	332	-5.296	-8.960	28.652	1.00	23.83
ATOM	1318	CD2	LEU	332	-6.897	-7.041	28.509	1.00	23.83



ATOM	1319	C	LEU	332	-9.630	-9.039	31.091	1.00	31.47
ATOM	1320	O	LEU	332	-9.665	-9.969	31.895	1.00	23.83
ATOM	1321	N	LEU	333	-10.659	-8.702	30.321	1.00	27.66
ATOM	1322	CA	LEU	333	-11.927	-9.422	30.351	1.00	27.66
ATOM	1323	CB	LEU	333	-13.072	-8.500	29.918	1.00	49.79
ATOM	1324	CG	LEU	333	-13.416	-7.312	30.820	1.00	49.79
ATOM	1325	CD1	LEU	333	-14.328	-6.339	30.083	1.00	49.79
ATOM	1326	CD2	LEU	333	-14.072	-7.803	32.104	1.00	49.79
ATOM	1327	C	LEU	333	-11.904	-10.663	29.456	1.00	27.66
ATOM	1328	O	LEU	333	-12.117	-11.780	29.919	1.00	49.79
ATOM	1329	N	CYS	334	-11.616	-10.464	28.174	1.00	29.56
ATOM	1330	CA	CYS	334	-11.583	-11.566	27.220	1.00	29.56
ATOM	1331	CB	CYS	334	-12.134	-11.106	25.865	1.00	47.01
ATOM	1332	SG	CYS	334	-13.888	-10.657	25.883	1.00	47.01
ATOM	1333	C	CYS	334	-10.187	-12.161	27.050	1.00	29.56
ATOM	1334	O	CYS	334	-9.652	-12.202	25.942	1.00	47.01
ATOM	1335	N	VAL	335	-9.617	-12.655	28.147	1.00	30.69
ATOM	1336	CA	VAL	335	-8.280	-13.250	28.132	1.00	30.69
ATOM	1337	CB	VAL	335	-7.913	-13.844	29.514	1.00	32.18
ATOM	1338	CG1	VAL	335	-6.517	-14.456	29.480	1.00	32.18
ATOM	1339	CG2	VAL	335	-7.988	-12.768	30.584	1.00	32.18
ATOM	1340	C	VAL	335	-8.120	-14.340	27.068	1.00	30.69
ATOM	1341	O	VAL	335	-7.149	-14.337	26.309	1.00	32.18
ATOM	1342	N	ASP	336	-9.079	-15.260	27.012	1.00	30.13
ATOM	1343	CA	ASP	336	-9.040	-16.360	26.052	1.00	30.13
ATOM	1344	CB	ASP	336	-10.218	-17.311	26.284	1.00	63.22
ATOM	1345	CG	ASP	336	-10.178	-18.528	25.370	1.00	63.22
ATOM	1346	OD1	ASP	336	-11.119	-18.700	24.565	1.00	63.22
ATOM	1347	OD2	ASP	336	-9.205	-19.311	25.452	1.00	63.22
ATOM	1348	C	ASP	336	-9.012	-15.903	24.594	1.00	30.13
ATOM	1349	O	ASP	336	-8.156	-16.339	23.823	1.00	63.22
ATOM	1350	N	LYS	337	-9.944	-15.027	24.223	1.00	26.63
ATOM	1351	CA	LYS	337	-10.024	-14.515	22.856	1.00	26.63
ATOM	1352	CB	LYS	337	-11.172	-13.516	22.729	1.00	21.38
ATOM	1353	C	LYS	337	-8.706	-13.865	22.438	1.00	26.63
ATOM	1354	O	LYS	337	-8.204	-14.110	21.338	1.00	21.38
ATOM	1355	N	ILE	338	-8.141	-13.060	23.334	1.00	24.65
ATOM	1356	CA	ILE	338	-6.879	-12.376	23.078	1.00	24.65
ATOM	1357	CB	ILE	338	-6.543	-11.380	24.215	1.00	20.45
ATOM	1358	CG2	ILE	338	-5.198	-10.719	23.966	1.00	20.45
ATOM	1359	CG1	ILE	338	-7.632	-10.308	24.308	1.00	20.45
ATOM	1360	CD1	ILE	338	-7.479	-9.374	25.486	1.00	20.45
ATOM	1361	C	ILE	338	-5.744	-13.388	22.911	1.00	24.65
ATOM	1362	O	ILE	338	-4.948	-13.288	21.974	1.00	20.45
ATOM	1363	N	GLU	339	-5.700	-14.383	23.795	1.00	35.34
ATOM	1364	CA	GLU						

ATOM	1366	C	GLU	339	-4.744	-16.180	22.421	1.00	35.34
ATOM	1367	O	GLU	339	-3.720	-16.421	21.777	1.00	29.51
ATOM	1368	N	LYS	340	-5.959	-16.536	22.009	1.00	24.19
ATOM	1369	CA	LYS	340	-6.168	-17.256	20.755	1.00	24.19
ATOM	1370	CB	LYS	340	-7.627	-17.671	20.624	1.00	23.97
ATOM	1371	C	LYS	340	-5.754	-16.377	19.576	1.00	24.19
ATOM	1372	O	LYS	340	-5.197	-16.860	18.586	1.00	23.97
ATOM	1373	N	SER	341	-6.000	-15.079	19.708	1.00	16.85
ATOM	1374	CA	SER	341	-5.651	-14.115	18.676	1.00	16.85
ATOM	1375	CB	SER	341	-6.223	-12.744	19.033	1.00	26.59
ATOM	1376	OG	SER	341	-5.852	-11.765	18.080	1.00	26.59
ATOM	1377	C	SER	341	-4.137	-14.026	18.500	1.00	16.85
ATOM	1378	O	SER	341	-3.638	-14.042	17.374	1.00	26.59
ATOM	1379	N	GLN	342	-3.406	-13.932	19.608	1.00	17.35
ATOM	1380	CA	GLN	342	-1.952	-13.845	19.537	1.00	17.35
ATOM	1381	CB	GLN	342	-1.337	-13.597	20.913	1.00	30.07
ATOM	1382	CG	GLN	342	0.140	-13.245	20.832	1.00	30.07
ATOM	1383	CD	GLN	342	0.811	-13.196	22.182	1.00	30.07
ATOM	1384	OE1	GLN	342	0.884	-14.201	22.884	1.00	30.07
ATOM	1385	NE2	GLN	342	1.318	-12.030	22.548	1.00	30.07
ATOM	1386	C	GLN	342	-1.368	-15.118	18.944	1.00	17.35
ATOM	1387	O	GLN	342	-0.405	-15.066	18.178	1.00	30.07
ATOM	1388	N	GLU	343	-1.949	-16.260	19.303	1.00	18.35
ATOM	1389	CA	GLU	343	-1.489	-17.546	18.791	1.00	18.35
ATOM	1390	CB	GLU	343	-2.308	-18.676	19.394	1.00	16.98
ATOM	1391	C	GLU	343	-1.603	-17.560	17.267	1.00	18.35
ATOM	1392	O	GLU	343	-0.699	-18.026	16.568	1.00	16.98
ATOM	1393	N	ALA	344	-2.706	-17.017	16.761	1.00	14.83
ATOM	1394	CA	ALA	344	-2.946	-16.948	15.324	1.00	14.83
ATOM	1395	CB	ALA	344	-4.327	-16.376	15.049	1.00	19.42
ATOM	1396	C	ALA	344	-1.872	-16.102	14.640	1.00	14.83
ATOM	1397	O	ALA	344	-1.311	-16.507	13.619	1.00	19.42
ATOM	1398	N	TYR	345	-1.586	-14.934	15.211	1.00	13.10
ATOM	1399	CA	TYR	345	-0.569	-14.041	14.665	1.00	13.10
ATOM	1400	CB	TYR	345	-0.573	-12.697	15.393	1.00	2.00
ATOM	1401	CG	TYR	345	-1.670	-11.767	14.938	1.00	2.00
ATOM	1402	CD1	TYR	345	-2.707	-11.409	15.794	1.00	2.00
ATOM	1403	CE1	TYR	345	-3.722	-10.562	15.377	1.00	2.00
ATOM	1404	CD2	TYR	345	-1.674	-11.248	13.647	1.00	2.00
ATOM	1405	CE2	TYR	345	-2.683	-10.398	13.219	1.00	2.00
ATOM	1406	CZ	TYR	345	-3.706	-10.061	14.087	1.00	2.00
ATOM	1407	OH	TYR	345	-4.722	-9.233	13.669	1.00	2.00
ATOM	1408	C	TYR	345	0.818	-14.666	14.732	1.00	13.10
ATOM	1409	O	TYR	345	1.614	-14.504	13.811	1.00	2.00
ATOM	1410	N	LEU	346	1.101	-15.387	15.813	1.00	12.59
ATOM	1411	CA	LEU	346					

ATOM	1413	CG	LEU	346	2.899	-15.799	18.504	1.00	22.61
ATOM	1414	CD1	LEU	346	2.717	-16.511	19.830	1.00	22.61
ATOM	1415	CD2	LEU	346	4.341	-15.357	18.324	1.00	22.61
ATOM	1416	C	LEU	346	2.629	-17.057	14.865	1.00	12.59
ATOM	1417	O	LEU	346	3.706	-17.099	14.272	1.00	22.61
ATOM	1418	N	LEU	347	1.612	-17.862	14.574	1.00	18.42
ATOM	1419	CA	LEU	347	1.706	-18.863	13.517	1.00	18.42
ATOM	1420	CB	LEU	347	0.471	-19.762	13.512	1.00	23.56
ATOM	1421	CG	LEU	347	0.509	-20.965	14.456	1.00	23.56
ATOM	1422	CD1	LEU	347	-0.819	-21.702	14.398	1.00	23.56
ATOM	1423	CD2	LEU	347	1.659	-21.890	14.068	1.00	23.56
ATOM	1424	C	LEU	347	1.870	-18.201	12.154	1.00	18.42
ATOM	1425	O	LEU	347	2.672	-18.651	11.330	1.00	23.56
ATOM	1426	N	ALA	348	1.099	-17.144	11.917	1.00	12.49
ATOM	1427	CA	ALA	348	1.157	-16.403	10.663	1.00	12.49
ATOM	1428	CB	ALA	348	0.098	-15.302	10.654	1.00	14.77
ATOM	1429	C	ALA	348	2.545	-15.798	10.504	1.00	12.49
ATOM	1430	O	ALA	348	3.154	-15.874	9.436	1.00	14.77
ATOM	1431	N	PHE	349	3.048	-15.246	11.602	1.00	15.52
ATOM	1432	CA	PHE	349	4.357	-14.613	11.664	1.00	15.52
ATOM	1433	CB	PHE	349	4.566	-14.049	13.076	1.00	14.41
ATOM	1434	CG	PHE	349	5.714	-13.085	13.203	1.00	14.41
ATOM	1435	CD1	PHE	349	6.473	-12.712	12.099	1.00	14.41
ATOM	1436	CD2	PHE	349	6.027	-12.540	14.443	1.00	14.41
ATOM	1437	CE1	PHE	349	7.523	-11.813	12.230	1.00	14.41
ATOM	1438	CE2	PHE	349	7.075	-11.640	14.584	1.00	14.41
ATOM	1439	CZ	PHE	349	7.825	-11.275	13.475	1.00	14.41
ATOM	1440	C	PHE	349	5.444	-15.633	11.324	1.00	15.52
ATOM	1441	O	PHE	349	6.252	-15.413	10.422	1.00	14.41
ATOM	1442	N	GLU	350	5.439	-16.760	12.026	1.00	13.20
ATOM	1443	CA	GLU	350	6.424	-17.811	11.801	1.00	13.20
ATOM	1444	CB	GLU	350	6.152	-18.995	12.734	1.00	33.43
ATOM	1445	CG	GLU	350	7.068	-20.193	12.519	1.00	33.43
ATOM	1446	CD	GLU	350	6.786	-21.331	13.482	1.00	33.43
ATOM	1447	OE1	GLU	350	7.746	-22.035	13.857	1.00	33.43
ATOM	1448	OE2	GLU	350	5.611	-21.525	13.865	1.00	33.43
ATOM	1449	C	GLU	350	6.409	-18.283	10.352	1.00	13.20
ATOM	1450	O	GLU	350	7.449	-18.355	9.694	1.00	33.43
ATOM	1451	N	HIS	351	5.217	-18.573	9.850	1.00	19.10
ATOM	1452	CA	HIS	351	5.062	-19.051	8.485	1.00	19.10
ATOM	1453	CB	HIS	351	3.632	-19.536	8.256	1.00	18.97
ATOM	1454	CG	HIS	351	3.249	-20.700	9.117	1.00	18.97
ATOM	1455	CD2	HIS	351	3.987	-21.474	9.948	1.00	18.97
ATOM	1456	ND1	HIS	351	1.960	-21.180	9.194	1.00	18.97
ATOM	1457	CE1	HIS	351	1.918	-22.195	10.039	1.00	18.97
ATOM	1458	NE2	HIS	351	3.134	-22.394	10.509	1.00	18.97
ATOM	1459	C	HIS	351	5.477	-18.011	7.449	1.00	19.10

ATOM	1460	O	HIS	351	5.955	-18.366	6.371	1.00	18.97
ATOM	1461	N	TYR	352	5.304	-16.732	7.767	1.00	9.38
ATOM	1462	CA	TYR	352	5.711	-15.683	6.843	1.00	9.38
ATOM	1463	CB	TYR	352	5.168	-14.317	7.257	1.00	16.06
ATOM	1464	CG	TYR	352	5.539	-13.238	6.268	1.00	16.06
ATOM	1465	CD1	TYR	352	4.939	-13.190	5.008	1.00	16.06
ATOM	1466	CE1	TYR	352	5.321	-12.242	4.060	1.00	16.06
ATOM	1467	CD2	TYR	352	6.531	-12.303	6.562	1.00	16.06
ATOM	1468	CE2	TYR	352	6.923	-11.349	5.620	1.00	16.06
ATOM	1469	CZ	TYR	352	6.313	-11.326	4.371	1.00	16.06
ATOM	1470	OH	TYR	352	6.710	-10.401	3.431	1.00	16.06
ATOM	1471	C	TYR	352	7.234	-15.639	6.812	1.00	9.38
ATOM	1472	O	TYR	352	7.838	-15.475	5.751	1.00	16.06
ATOM	1473	N	VAL	353	7.851	-15.789	7.980	1.00	15.38
ATOM	1474	CA	VAL	353	9.305	-15.790	8.087	1.00	15.38
ATOM	1475	CB	VAL	353	9.761	-15.945	9.558	1.00	18.40
ATOM	1476	CG1	VAL	353	11.262	-16.163	9.633	1.00	18.40
ATOM	1477	CG2	VAL	353	9.384	-14.703	10.349	1.00	18.40
ATOM	1478	C	VAL	353	9.853	-16.938	7.237	1.00	15.38
ATOM	1479	O	VAL	353	10.850	-16.773	6.525	1.00	18.40
ATOM	1480	N	ASN	354	9.183	-18.086	7.298	1.00	14.74
ATOM	1481	CA	ASN	354	9.578	-19.259	6.521	1.00	14.74
ATOM	1482	CB	ASN	354	8.640	-20.435	6.799	1.00	19.97
ATOM	1483	CG	ASN	354	8.832	-21.020	8.180	1.00	19.97
ATOM	1484	OD1	ASN	354	9.879	-20.848	8.799	1.00	19.97
ATOM	1485	ND2	ASN	354	7.826	-21.734	8.664	1.00	19.97
ATOM	1486	C	ASN	354	9.550	-18.939	5.034	1.00	14.74
ATOM	1487	O	ASN	354	10.452	-19.319	4.290	1.00	19.97
ATOM	1488	N	HIS	355	8.507	-18.230	4.613	1.00	13.03
ATOM	1489	CA	HIS	355	8.329	-17.837	3.220	1.00	13.03
ATOM	1490	CB	HIS	355	6.960	-17.164	3.042	1.00	24.39
ATOM	1491	CG	HIS	355	6.753	-16.541	1.695	1.00	24.39
ATOM	1492	CD2	HIS	355	7.195	-15.370	1.176	1.00	24.39
ATOM	1493	ND1	HIS	355	6.009	-17.138	0.701	1.00	24.39
ATOM	1494	CE1	HIS	355	6.005	-16.368	-0.372	1.00	24.39
ATOM	1495	NE2	HIS	355	6.720	-15.289	-0.107	1.00	24.39
ATOM	1496	C	HIS	355	9.434	-16.894	2.758	1.00	13.03
ATOM	1497	O	HIS	355	9.834	-16.920	1.595	1.00	24.39
ATOM	1498	N	ARG	356	9.878	-16.027	3.660	1.00	19.55
ATOM	1499	CA	ARG	356	10.920	-15.054	3.358	1.00	19.55
ATOM	1500	CB	ARG	356	10.970	-14.001	4.460	1.00	22.01
ATOM	1501	CG	ARG	356	9.772	-13.081	4.454	1.00	22.01
ATOM	1502	CD	ARG	356	10.097	-11.784	3.750	1.00	22.01
ATOM	1503	NE	ARG	356	10.932	-10.934	4.592	1.00	22.01
ATOM	1504	CZ	ARG	356	11.822	-10.059	4.137	1.00	22.01
ATOM	1505	NH1	ARG	356	12.010	-9.907	2.833	1.	



ATOM	1507	C	ARG	356	12.297	-15.675	3.158	1.00	19.55
ATOM	1508	O	ARG	356	13.127	-15.126	2.434	1.00	22.01
ATOM	1509	N	LYS	357	12.547	-16.788	3.841	1.00	23.18
ATOM	1510	CA	LYS	357	13.815	-17.504	3.739	1.00	23.18
ATOM	1511	CB	LYS	357	13.879	-18.273	2.415	1.00	42.91
ATOM	1512	CG	LYS	357	12.750	-19.277	2.274	1.00	42.91
ATOM	1513	CD	LYS	357	12.773	-20.021	0.960	1.00	42.91
ATOM	1514	CE	LYS	357	11.619	-21.011	0.913	1.00	42.91
ATOM	1515	NZ	LYS	357	11.629	-21.845	-0.316	1.00	42.91
ATOM	1516	C	LYS	357	15.047	-16.619	3.918	1.00	23.18
ATOM	1517	O	LYS	357	15.816	-16.396	2.982	1.00	42.91
ATOM	1518	N	HIS	358	15.228	-16.122	5.137	1.00	32.39
ATOM	1519	CA	HIS	358	16.367	-15.272	5.460	1.00	32.39
ATOM	1520	CB	HIS	358	16.181	-14.626	6.835	1.00	26.77
ATOM	1521	CG	HIS	358	15.232	-13.468	6.841	1.00	26.77
ATOM	1522	CD2	HIS	358	15.452	-12.138	6.709	1.00	26.77
ATOM	1523	ND1	HIS	358	13.875	-13.615	7.028	1.00	26.77
ATOM	1524	CE1	HIS	358	13.300	-12.426	7.012	1.00	26.77
ATOM	1525	NE2	HIS	358	14.234	-11.513	6.821	1.00	26.77
ATOM	1526	C	HIS	358	17.633	-16.115	5.480	1.00	32.39
ATOM	1527	O	HIS	358	17.618	-17.248	5.961	1.00	26.77
ATOM	1528	N	ASN	359	18.728	-15.561	4.972	1.00	41.97
ATOM	1529	CA	ASN	359	20.000	-16.273	4.959	1.00	41.97
ATOM	1530	CB	ASN	359	20.909	-15.716	3.863	1.00	46.84
ATOM	1531	C	ASN	359	20.663	-16.134	6.331	1.00	41.97
ATOM	1532	O	ASN	359	21.821	-15.731	6.436	1.00	46.84
ATOM	1533	N	ILE	360	19.908	-16.450	7.379	1.00	35.72
ATOM	1534	CA	ILE	360	20.394	-16.359	8.753	1.00	35.72
ATOM	1535	CB	ILE	360	19.819	-15.113	9.480	1.00	36.14
ATOM	1536	CG2	ILE	360	20.327	-15.050	10.918	1.00	36.14
ATOM	1537	CG1	ILE	360	20.204	-13.833	8.734	1.00	36.14
ATOM	1538	CD1	ILE	360	19.526	-12.591	9.265	1.00	36.14
ATOM	1539	C	ILE	360	19.935	-17.611	9.493	1.00	35.72
ATOM	1540	O	ILE	360	18.748	-17.953	9.479	1.00	36.14
ATOM	1541	N	PRO	361	20.877	-18.338	10.109	1.00	31.56
ATOM	1542	CD	PRO	361	22.334	-18.114	10.100	1.00	33.50
ATOM	1543	CA	PRO	361	20.532	-19.556	10.847	1.00	31.56
ATOM	1544	CB	PRO	361	21.901	-20.163	11.161	1.00	33.50
ATOM	1545	CG	PRO	361	22.801	-18.967	11.249	1.00	33.50
ATOM	1546	C	PRO	361	19.743	-19.256	12.121	1.00	31.56
ATOM	1547	O	PRO	361	20.080	-18.338	12.867	1.00	33.50
ATOM	1548	N	HIS	362	18.688	-20.034	12.355	1.00	18.84
ATOM	1549	CA	HIS	362	17.840	-19.887	13.541	1.00	18.84
ATOM	1550	CB	HIS	362	18.656	-20.151	14.812	1.00	31.38
ATOM	1551	CG	HIS	362	19.540	-21.357	14.731	1.00	31.38
ATOM	1552	CD2	HIS	36					



ATOM	1554	CE1 HIS	362	21.427	-22.497	14.754	1.00	31.38
ATOM	1555	NE2 HIS	362	20.439	-23.353	14.558	1.00	31.38
ATOM	1556	C HIS	362	17.189	-18.506	13.628	1.00	18.84
ATOM	1557	O HIS	362	16.980	-17.979	14.723	1.00	31.38
ATOM	1558	N PHE	363	16.825	-17.950	12.476	1.00	18.69
ATOM	1559	CA PHE	363	16.209	-16.630	12.408	1.00	18.69
ATOM	1560	CB PHE	363	15.825	-16.302	10.962	1.00	19.25
ATOM	1561	CG PHE	363	15.339	-14.894	10.765	1.00	19.25
ATOM	1562	CD1 PHE	363	16.239	-13.862	10.530	1.00	19.25
ATOM	1563	CD2 PHE	363	13.981	-14.598	10.819	1.00	19.25
ATOM	1564	CE1 PHE	363	15.794	-12.556	10.351	1.00	19.25
ATOM	1565	CE2 PHE	363	13.527	-13.296	10.642	1.00	19.25
ATOM	1566	CZ PHE	363	14.435	-12.273	10.407	1.00	19.25
ATOM	1567	C PHE	363	14.995	-16.461	13.323	1.00	18.69
ATOM	1568	O PHE	363	14.955	-15.540	14.138	1.00	19.25
ATOM	1569	N TRP	364	14.016	-17.351	13.191	1.00	16.46
ATOM	1570	CA TRP	364	12.797	-17.280	13.995	1.00	16.46
ATOM	1571	CB TRP	364	11.882	-18.482	13.706	1.00	17.81
ATOM	1572	CG TRP	364	10.588	-18.488	14.481	1.00	17.81
ATOM	1573	CD2 TRP	364	9.586	-17.458	14.504	1.00	17.81
ATOM	1574	CE2 TRP	364	8.547	-17.905	15.350	1.00	17.81
ATOM	1575	CE3 TRP	364	9.467	-16.202	13.894	1.00	17.81
ATOM	1576	CD1 TRP	364	10.126	-19.486	15.290	1.00	17.81
ATOM	1577	NE1 TRP	364	8.902	-19.144	15.814	1.00	17.81
ATOM	1578	CZ2 TRP	364	7.403	-17.142	15.602	1.00	17.81
ATOM	1579	CZ3 TRP	364	8.329	-15.444	14.145	1.00	17.81
ATOM	1580	CH2 TRP	364	7.312	-15.919	14.992	1.00	17.81
ATOM	1581	C TRP	364	13.046	-17.114	15.500	1.00	16.46
ATOM	1582	O TRP	364	12.595	-16.133	16.087	1.00	17.81
ATOM	1583	N PRO	365	13.779	-18.051	16.137	1.00	18.31
ATOM	1584	CD PRO	365	14.342	-19.314	15.625	1.00	25.61
ATOM	1585	CA PRO	365	14.038	-17.920	17.577	1.00	18.31
ATOM	1586	CB PRO	365	14.939	-19.118	17.874	1.00	25.61
ATOM	1587	CG PRO	365	14.500	-20.130	16.882	1.00	25.61
ATOM	1588	C PRO	365	14.732	-16.606	17.933	1.00	18.31
ATOM	1589	O PRO	365	14.387	-15.963	18.926	1.00	25.61
ATOM	1590	N LYS	366	15.699	-16.207	17.112	1.00	25.16
ATOM	1591	CA LYS	366	16.439	-14.968	17.338	1.00	25.16
ATOM	1592	CB LYS	366	17.537	-14.805	16.289	1.00	40.51
ATOM	1593	CG LYS	366	18.679	-15.792	16.417	1.00	40.51
ATOM	1594	CD LYS	366	19.664	-15.607	15.278	1.00	40.51
ATOM	1595	CE LYS	366	20.884	-16.492	15.440	1.00	40.51
ATOM	1596	NZ LYS	366	21.800	-16.360	14.275	1.00	40.51
ATOM	1597	C LYS	366	15.521	-13.747	17.317	1.00	25.16
ATOM	1598	O LYS	366	15.593	-12.893	18.202	1.00	40.51
ATOM	1599	N LEU	367	14.661	-13.666	16.307	1.00	25.30
ATOM	1600	CA LEU	367	13.729	-12.551	16.184	1.00	25.30

ATOM	1601	CB	LEU	367	12.989	-12.620	14.845	1.00	27.80
ATOM	1602	CG	LEU	367	11.964	-11.519	14.561	1.00	27.80
ATOM	1603	CD1	LEU	367	12.621	-10.147	14.679	1.00	27.80
ATOM	1604	CD2	LEU	367	11.367	-11.724	13.175	1.00	27.80
ATOM	1605	C	LEU	367	12.730	-12.596	17.332	1.00	25.30
ATOM	1606	O	LEU	367	12.337	-11.563	17.877	1.00	27.80
ATOM	1607	N	LEU	368	12.345	-13.807	17.712	1.00	26.12
ATOM	1608	CA	LEU	368	11.396	-14.019	18.793	1.00	26.12
ATOM	1609	CB	LEU	368	11.105	-15.515	18.919	1.00	33.27
ATOM	1610	CG	LEU	368	9.696	-15.976	19.289	1.00	33.27
ATOM	1611	CD1	LEU	368	8.640	-15.182	18.529	1.00	33.27
ATOM	1612	CD2	LEU	368	9.582	-17.460	18.976	1.00	33.27
ATOM	1613	C	LEU	368	11.973	-13.466	20.096	1.00	26.12
ATOM	1614	O	LEU	368	11.249	-12.920	20.930	1.00	33.27
ATOM	1615	N	MET	369	13.289	-13.571	20.244	1.00	24.39
ATOM	1616	CA	MET	369	13.971	-13.076	21.432	1.00	24.39
ATOM	1617	CB	MET	369	15.382	-13.656	21.511	1.00	47.44
ATOM	1618	CG	MET	369	15.407	-15.096	22.009	1.00	47.44
ATOM	1619	SD	MET	369	16.850	-16.029	21.464	1.00	47.44
ATOM	1620	CE	MET	369	18.186	-15.114	22.246	1.00	47.44
ATOM	1621	C	MET	369	13.996	-11.552	21.491	1.00	24.39
ATOM	1622	O	MET	369	14.212	-10.971	22.557	1.00	47.44
ATOM	1623	N	LYS	370	13.749	-10.904	20.354	1.00	27.31
ATOM	1624	CA	LYS	370	13.713	-9.445	20.297	1.00	27.31
ATOM	1625	CB	LYS	370	13.739	-8.951	18.847	1.00	28.20
ATOM	1626	CG	LYS	370	15.004	-9.312	18.090	1.00	28.20
ATOM	1627	CD	LYS	370	16.231	-8.810	18.824	1.00	28.20
ATOM	1628	CE	LYS	370	17.512	-9.244	18.142	1.00	28.20
ATOM	1629	NZ	LYS	370	18.696	-8.851	18.952	1.00	28.20
ATOM	1630	C	LYS	370	12.453	-8.945	21.002	1.00	27.31
ATOM	1631	O	LYS	370	12.424	-7.835	21.535	1.00	28.20
ATOM	1632	N	VAL	371	11.413	-9.776	21.009	1.00	26.41
ATOM	1633	CA	VAL	371	10.157	-9.432	21.668	1.00	26.41
ATOM	1634	CB	VAL	371	9.109	-10.561	21.512	1.00	25.61
ATOM	1635	CG1	VAL	371	7.825	-10.205	22.245	1.00	25.61
ATOM	1636	CG2	VAL	371	8.819	-10.805	20.044	1.00	25.61
ATOM	1637	C	VAL	371	10.450	-9.205	23.151	1.00	26.41
ATOM	1638	O	VAL	371	9.962	-8.248	23.752	1.00	25.61
ATOM	1639	N	THR	372	11.294	-10.065	23.713	1.00	26.28
ATOM	1640	CA	THR	372	11.683	-9.972	25.116	1.00	26.28
ATOM	1641	CB	THR	372	12.656	-11.109	25.500	1.00	28.14
ATOM	1642	OG1	THR	372	12.025	-12.377	25.275	1.00	28.14
ATOM	1643	CG2	THR	372	13.055	-11.001	26.965	1.00	28.14
ATOM	1644	C	THR	372	12.358	-8.624	25.372	1.00	26.28
ATOM	1645	O	THR	372	12.047	-7.937	26.350	1.00	28.14
ATOM									

ATOM	1648	CB	ASP	373	14.976	-6.822	23.435	1.00	37.94
ATOM	1649	CG	ASP	373	16.065	-7.893	23.445	1.00	37.94
ATOM	1650	OD1	ASP	373	16.248	-8.571	24.483	1.00	37.94
ATOM	1651	OD2	ASP	373	16.750	-8.052	22.410	1.00	37.94
ATOM	1652	C	ASP	373	12.969	-5.833	24.577	1.00	15.09
ATOM	1653	O	ASP	373	13.040	-4.928	25.407	1.00	37.94
ATOM	1654	N	LEU	374	12.008	-5.901	23.659	1.00	17.04
ATOM	1655	CA	LEU	374	10.974	-4.880	23.549	1.00	17.04
ATOM	1656	CB	LEU	374	10.071	-5.155	22.344	1.00	20.58
ATOM	1657	CG	LEU	374	10.624	-4.720	20.985	1.00	20.58
ATOM	1658	CD1	LEU	374	9.826	-5.352	19.862	1.00	20.58
ATOM	1659	CD2	LEU	374	10.599	-3.202	20.882	1.00	20.58
ATOM	1660	C	LEU	374	10.145	-4.786	24.825	1.00	17.04
ATOM	1661	O	LEU	374	9.783	-3.688	25.256	1.00	20.58
ATOM	1662	N	ARG	375	9.850	-5.935	25.430	1.00	20.46
ATOM	1663	CA	ARG	375	9.080	-5.977	26.673	1.00	20.46
ATOM	1664	CB	ARG	375	8.873	-7.422	27.140	1.00	55.89
ATOM	1665	CG	ARG	375	8.180	-8.354	26.152	1.00	55.89
ATOM	1666	CD	ARG	375	6.692	-8.084	26.027	1.00	55.89
ATOM	1667	NE	ARG	375	5.943	-9.338	25.968	1.00	55.89
ATOM	1668	CZ	ARG	375	5.054	-9.654	25.028	1.00	55.89
ATOM	1669	NH1	ARG	375	4.782	-8.808	24.040	1.00	55.89
ATOM	1670	NH2	ARG	375	4.438	-10.829	25.073	1.00	55.89
ATOM	1671	C	ARG	375	9.874	-5.221	27.735	1.00	20.46
ATOM	1672	O	ARG	375	9.328	-4.391	28.463	1.00	55.89
ATOM	1673	N	MET	376	11.174	-5.502	27.794	1.00	20.10
ATOM	1674	CA	MET	376	12.076	-4.863	28.744	1.00	20.10
ATOM	1675	CB	MET	376	13.493	-5.417	28.580	1.00	63.73
ATOM	1676	CG	MET	376	13.956	-6.310	29.722	1.00	63.73
ATOM	1677	SD	MET	376	14.494	-5.373	31.182	1.00	63.73
ATOM	1678	CE	MET	376	12.934	-5.151	32.087	1.00	63.73
ATOM	1679	C	MET	376	12.081	-3.347	28.566	1.00	20.10
ATOM	1680	O	MET	376	11.973	-2.602	29.539	1.00	63.73
ATOM	1681	N	ILE	377	12.194	-2.896	27.321	1.00	30.02
ATOM	1682	CA	ILE	377	12.198	-1.469	27.014	1.00	30.02
ATOM	1683	CB	ILE	377	12.329	-1.228	25.488	1.00	19.31
ATOM	1684	CG2	ILE	377	12.088	0.242	25.152	1.00	19.31
ATOM	1685	CG1	ILE	377	13.711	-1.685	25.011	1.00	19.31
ATOM	1686	CD1	ILE	377	13.906	-1.634	23.507	1.00	19.31
ATOM	1687	C	ILE	377	10.915	-0.821	27.542	1.00	30.02
ATOM	1688	O	ILE	377	10.962	0.216	28.211	1.00	19.31
ATOM	1689	N	GLY	378	9.779	-1.455	27.266	1.00	21.85
ATOM	1690	CA	GLY	378	8.505	-0.936	27.729	1.00	21.85
ATOM	1691	C	GLY	378	8.459	-0.821	29.243	1.00	21.85
ATOM	1692	O	GLY	378	7.990	0.185	29.779	1.00	34.01
ATOM	1693	N	ALA	379	8.967	-1.842			

ATOM	1695	CB	ALA	379	9.471	-3.231	31.880	1.00	30.06
ATOM	1696	C	ALA	379	9.895	-0.763	31.938	1.00	31.30
ATOM	1697	O	ALA	379	9.482	0.002	32.810	1.00	30.06
ATOM	1698	N	CYS	380	11.117	-0.677	31.418	1.00	28.61
ATOM	1699	CA	CYS	380	12.067	0.349	31.841	1.00	28.61
ATOM	1700	CB	CYS	380	13.360	0.268	31.025	1.00	60.26
ATOM	1701	SG	CYS	380	14.499	-1.067	31.470	1.00	60.26
ATOM	1702	C	CYS	380	11.449	1.730	31.658	1.00	28.61
ATOM	1703	O	CYS	380	11.516	2.573	32.554	1.00	60.26
ATOM	1704	N	HIS	381	10.840	1.957	30.498	1.00	30.42
ATOM	1705	CA	HIS	381	10.212	3.243	30.216	1.00	30.42
ATOM	1706	CB	HIS	381	9.696	3.306	28.779	1.00	16.49
ATOM	1707	CG	HIS	381	8.942	4.562	28.472	1.00	16.49
ATOM	1708	CD2	HIS	381	9.370	5.805	28.151	1.00	16.49
ATOM	1709	ND1	HIS	381	7.566	4.633	28.524	1.00	16.49
ATOM	1710	CE1	HIS	381	7.180	5.866	28.251	1.00	16.49
ATOM	1711	NE2	HIS	381	8.255	6.596	28.021	1.00	16.49
ATOM	1712	C	HIS	381	9.073	3.539	31.182	1.00	30.42
ATOM	1713	O	HIS	381	8.856	4.690	31.552	1.00	16.49
ATOM	1714	N	ALA	382	8.330	2.506	31.564	1.00	22.89
ATOM	1715	CA	ALA	382	7.218	2.666	32.493	1.00	22.89
ATOM	1716	CB	ALA	382	6.520	1.336	32.708	1.00	34.50
ATOM	1717	C	ALA	382	7.738	3.213	33.819	1.00	22.89
ATOM	1718	O	ALA	382	7.219	4.200	34.343	1.00	34.50
ATOM	1719	N	SER	383	8.789	2.586	34.336	1.00	26.39
ATOM	1720	CA	SER	383	9.400	3.006	35.591	1.00	26.39
ATOM	1721	CB	SER	383	10.510	2.030	35.985	1.00	52.94
ATOM	1722	OG	SER	383	10.015	0.702	36.046	1.00	52.94
ATOM	1723	C	SER	383	9.966	4.418	35.470	1.00	26.39
ATOM	1724	O	SER	383	9.772	5.253	36.357	1.00	52.94
ATOM	1725	N	ARG	384	10.662	4.683	34.368	1.00	30.36
ATOM	1726	CA	ARG	384	11.249	5.995	34.134	1.00	30.36
ATOM	1727	CB	ARG	384	12.116	5.977	32.874	1.00	37.39
ATOM	1728	CG	ARG	384	12.601	7.344	32.431	1.00	37.39
ATOM	1729	CD	ARG	384	14.070	7.321	32.060	1.00	37.39
ATOM	1730	NE	ARG	384	14.935	7.597	33.204	1.00	37.39
ATOM	1731	CZ	ARG	384	15.750	8.646	33.291	1.00	37.39
ATOM	1732	NH1	ARG	384	15.824	9.529	32.303	1.00	37.39
ATOM	1733	NH2	ARG	384	16.488	8.819	34.376	1.00	37.39
ATOM	1734	C	ARG	384	10.169	7.067	34.030	1.00	30.36
ATOM	1735	O	ARG	384	10.301	8.144	34.616	1.00	37.39
ATOM	1736	N	PHE	385	9.078	6.749	33.338	1.00	24.47
ATOM	1737	CA	PHE	385	7.980	7.693	33.171	1.00	24.47
ATOM	1738	CB	PHE	385	6.859	7.092	32.319	1.00	28.70
ATOM	1739	CG	PHE	385	5.710	8.036	32.075	1.00	28.70
ATOM	1740	CD1	PHE	385	5.795	9.017	31.092	1.00	28.70
ATOM	1741	CD2	PHE	385	4.549	7.954	32.836	1.00	28.70



ATOM	1742	CE1 PHE	385	4.740	9.903	30.874	1.00	28.70
ATOM	1743	CE2 PHE	385	3.491	8.835	32.624	1.00	28.70
ATOM	1744	CZ PHE	385	3.587	9.812	31.641	1.00	28.70
ATOM	1745	C PHE	385	7.436	8.097	34.533	1.00	24.47
ATOM	1746	O PHE	385	7.250	9.285	34.805	1.00	28.70
ATOM	1747	N LEU	386	7.208	7.107	35.391	1.00	31.13
ATOM	1748	CA LEU	386	6.690	7.352	36.734	1.00	31.13
ATOM	1749	CB LEU	386	6.596	6.044	37.513	1.00	39.10
ATOM	1750	C LEU	386	7.577	8.348	37.474	1.00	31.13
ATOM	1751	O LEU	386	7.085	9.201	38.217	1.00	39.10
ATOM	1752	N HIS	387	8.884	8.254	37.243	1.00	36.46
ATOM	1753	CA HIS	387	9.837	9.152	37.881	1.00	36.46
ATOM	1754	CB HIS	387	11.258	8.589	37.794	1.00	62.78
ATOM	1755	CG HIS	387	11.459	7.338	38.590	1.00	62.78
ATOM	1756	CD2 HIS	387	10.601	6.614	39.346	1.00	62.78
ATOM	1757	ND1 HIS	387	12.675	6.689	38.663	1.00	62.78
ATOM	1758	CE1 HIS	387	12.554	5.620	39.431	1.00	62.78
ATOM	1759	NE2 HIS	387	11.309	5.550	39.856	1.00	62.78
ATOM	1760	C HIS	387	9.778	10.544	37.266	1.00	36.46
ATOM	1761	O HIS	387	9.885	11.543	37.979	1.00	62.78
ATOM	1762	N MET	388	9.587	10.612	35.950	1.00	33.41
ATOM	1763	CA MET	388	9.505	11.894	35.258	1.00	33.41
ATOM	1764	CB MET	388	9.269	11.703	33.755	1.00	42.63
ATOM	1765	CG MET	388	10.456	11.144	32.982	1.00	42.63
ATOM	1766	SD MET	388	10.253	11.325	31.192	1.00	42.63
ATOM	1767	CE MET	388	9.501	9.772	30.748	1.00	42.63
ATOM	1768	C MET	388	8.385	12.746	35.849	1.00	33.41
ATOM	1769	O MET	388	8.573	13.934	36.103	1.00	42.63
ATOM	1770	N LYS	389	7.235	12.126	36.092	1.00	39.26
ATOM	1771	CA LYS	389	6.082	12.825	36.659	1.00	39.26
ATOM	1772	CB LYS	389	4.867	11.900	36.719	1.00	52.87
ATOM	1773	CG LYS	389	4.237	11.594	35.379	1.00	52.87
ATOM	1774	CD LYS	389	3.048	10.667	35.553	1.00	52.87
ATOM	1775	CE LYS	389	3.482	9.327	36.125	1.00	52.87
ATOM	1776	NZ LYS	389	2.335	8.407	36.326	1.00	52.87
ATOM	1777	C LYS	389	6.363	13.360	38.056	1.00	39.26
ATOM	1778	O LYS	389	5.837	14.404	38.452	1.00	52.87
ATOM	1779	N VAL	390	7.156	12.614	38.818	1.00	44.18
ATOM	1780	CA VAL	390	7.508	13.016	40.172	1.00	44.18
ATOM	1781	CB VAL	390	8.299	11.898	40.905	1.00	50.50
ATOM	1782	CG1 VAL	390	8.718	12.362	42.293	1.00	50.50
ATOM	1783	CG2 VAL	390	7.455	10.640	41.012	1.00	50.50
ATOM	1784	C VAL	390	8.352	14.288	40.145	1.00	44.18
ATOM	1785	O VAL	390	8.144	15.198	40.948	1.00	50.50
ATOM	1786	N GLU	391	9.261	14.368	39.179	1.00	38.64
ATOM	1787	CA GLU	391	10.161	15.509	39.056	1.00	38.64
ATOM	1788	CB GLU	391	11.483	15.060	38.424	1.00	64.18



ATOM	1789	CG	GLU	391	12.065	13.766	39.009	1.00	64.18
ATOM	1790	CD	GLU	391	12.662	13.922	40.405	1.00	64.18
ATOM	1791	OE1	GLU	391	12.190	14.773	41.192	1.00	64.18
ATOM	1792	OE2	GLU	391	13.611	13.173	40.721	1.00	64.18
ATOM	1793	C	GLU	391	9.623	16.737	38.314	1.00	38.64
ATOM	1794	O	GLU	391	9.656	17.850	38.849	1.00	64.18
ATOM	1795	N	CYS	392	9.125	16.539	37.096	1.00	37.24
ATOM	1796	CA	CYS	392	8.611	17.635	36.271	1.00	37.24
ATOM	1797	CB	CYS	392	8.879	17.345	34.784	1.00	30.64
ATOM	1798	SG	CYS	392	10.634	17.137	34.283	1.00	30.64
ATOM	1799	C	CYS	392	7.110	17.882	36.496	1.00	37.24
ATOM	1800	O	CYS	392	6.403	17.011	37.006	1.00	30.64
ATOM	1801	N	PRO	393	6.625	19.107	36.199	1.00	40.56
ATOM	1802	CD	PRO	393	7.444	20.297	35.904	1.00	33.41
ATOM	1803	CA	PRO	393	5.209	19.473	36.358	1.00	40.56
ATOM	1804	CB	PRO	393	5.253	21.001	36.404	1.00	33.41
ATOM	1805	CG	PRO	393	6.409	21.332	35.527	1.00	33.41
ATOM	1806	C	PRO	393	4.330	18.975	35.207	1.00	40.56
ATOM	1807	O	PRO	393	4.776	18.907	34.057	1.00	33.41
ATOM	1808	N	THR	394	3.067	18.691	35.516	1.00	41.91
ATOM	1809	CA	THR	394	2.101	18.186	34.540	1.00	41.91
ATOM	1810	CB	THR	394	0.691	18.075	35.156	1.00	62.04
ATOM	1811	OG1	THR	394	0.706	18.582	36.497	1.00	62.04
ATOM	1812	CG2	THR	394	0.232	16.626	35.168	1.00	62.04
ATOM	1813	C	THR	394	1.995	18.984	33.242	1.00	41.91
ATOM	1814	O	THR	394	1.758	18.411	32.181	1.00	62.04
ATOM	1815	N	GLU	395	2.191	20.297	33.327	1.00	43.92
ATOM	1816	CA	GLU	395	2.104	21.176	32.160	1.00	43.92
ATOM	1817	CB	GLU	395	2.313	22.626	32.585	1.00	34.22
ATOM	1818	C	GLU	395	3.071	20.814	31.031	1.00	43.92
ATOM	1819	O	GLU	395	2.887	21.243	29.891	1.00	34.22
ATOM	1820	N	LEU	396	4.104	20.041	31.350	1.00	34.92
ATOM	1821	CA	LEU	396	5.096	19.634	30.359	1.00	34.92
ATOM	1822	CB	LEU	396	6.473	19.495	31.017	1.00	35.81
ATOM	1823	CG	LEU	396	7.074	20.747	31.662	1.00	35.81
ATOM	1824	CD1	LEU	396	8.427	20.410	32.263	1.00	35.81
ATOM	1825	CD2	LEU	396	7.209	21.857	30.629	1.00	35.81
ATOM	1826	C	LEU	396	4.731	18.324	29.661	1.00	34.92
ATOM	1827	O	LEU	396	5.343	17.954	28.659	1.00	35.81
ATOM	1828	N	PHE	397	3.734	17.627	30.197	1.00	35.28
ATOM	1829	CA	PHE	397	3.302	16.352	29.640	1.00	35.28
ATOM	1830	CB	PHE	397	3.059	15.341	30.764	1.00	27.13
ATOM	1831	CG	PHE	397	4.285	15.004	31.561	1.00	27.13
ATOM	1832	CD1	PHE	397	4.700	15.824	32.604	1.00	27.13
ATOM	1833	CD2	PHE	397	5.021	13.860	31.273	1.00	27.13
ATOM	1834	CE1	PHE	397	5.831	15.510	33.349	1.00	27.13
ATOM	1835	CE2	PHE	397	6.155	13.537	32.013	1.00	27.13

ATOM	1836	CZ	PHE	397	6.561	14.364	33.052	1.00	27.13
ATOM	1837	C	PHE	397	2.027	16.474	28.812	1.00	35.28
ATOM	1838	O	PHE	397	0.977	16.861	29.331	1.00	27.13
ATOM	1839	N	PRO	398	2.102	16.164	27.505	1.00	26.41
ATOM	1840	CD	PRO	398	3.305	15.850	26.713	1.00	19.32
ATOM	1841	CA	PRO	398	0.917	16.247	26.647	1.00	26.41
ATOM	1842	CB	PRO	398	1.439	15.752	25.300	1.00	19.32
ATOM	1843	CG	PRO	398	2.867	16.193	25.312	1.00	19.32
ATOM	1844	C	PRO	398	-0.157	15.313	27.206	1.00	26.41
ATOM	1845	O	PRO	398	0.160	14.232	27.710	1.00	19.32
ATOM	1846	N	PRO	399	-1.439	15.702	27.104	1.00	25.12
ATOM	1847	CD	PRO	399	-1.935	16.929	26.454	1.00	24.32
ATOM	1848	CA	PRO	399	-2.554	14.894	27.612	1.00	25.12
ATOM	1849	CB	PRO	399	-3.777	15.594	27.022	1.00	24.32
ATOM	1850	CG	PRO	399	-3.349	17.026	26.974	1.00	24.32
ATOM	1851	C	PRO	399	-2.502	13.416	27.222	1.00	25.12
ATOM	1852	O	PRO	399	-2.599	12.540	28.085	1.00	24.32
ATOM	1853	N	LEU	400	-2.322	13.139	25.933	1.00	23.10
ATOM	1854	CA	LEU	400	-2.265	11.759	25.454	1.00	23.10
ATOM	1855	CB	LEU	400	-2.230	11.720	23.923	1.00	22.35
ATOM	1856	CG	LEU	400	-2.485	10.354	23.276	1.00	22.35
ATOM	1857	CD1	LEU	400	-3.792	9.765	23.792	1.00	22.35
ATOM	1858	CD2	LEU	400	-2.523	10.494	21.763	1.00	22.35
ATOM	1859	C	LEU	400	-1.066	11.012	26.032	1.00	23.10
ATOM	1860	O	LEU	400	-1.160	9.825	26.345	1.00	22.35
ATOM	1861	N	PHE	401	0.044	11.723	26.202	1.00	13.85
ATOM	1862	CA	PHE	401	1.269	11.150	26.755	1.00	13.85
ATOM	1863	CB	PHE	401	2.374	12.213	26.753	1.00	26.97
ATOM	1864	CG	PHE	401	3.729	11.702	27.164	1.00	26.97
ATOM	1865	CD1	PHE	401	4.189	10.461	26.732	1.00	26.97
ATOM	1866	CD2	PHE	401	4.561	12.481	27.963	1.00	26.97
ATOM	1867	CE1	PHE	401	5.459	10.005	27.091	1.00	26.97
ATOM	1868	CE2	PHE	401	5.830	12.035	28.327	1.00	26.97
ATOM	1869	CZ	PHE	401	6.280	10.795	27.889	1.00	26.97
ATOM	1870	C	PHE	401	0.993	10.659	28.179	1.00	13.85
ATOM	1871	O	PHE	401	1.393	9.558	28.555	1.00	26.97
ATOM	1872	N	LEU	402	0.274	11.473	28.947	1.00	25.21
ATOM	1873	CA	LEU	402	-0.080	11.145	30.325	1.00	25.21
ATOM	1874	CB	LEU	402	-0.640	12.380	31.035	1.00	29.34
ATOM	1875	CG	LEU	402	0.334	13.411	31.600	1.00	29.34
ATOM	1876	CD1	LEU	402	-0.430	14.658	32.018	1.00	29.34
ATOM	1877	CD2	LEU	402	1.090	12.814	32.775	1.00	29.34
ATOM	1878	C	LEU	402	-1.109	10.025	30.425	1.00	25.21
ATOM	1879	O	LEU	402	-1.034	9.189	31.320	1.00	29.34
ATOM	1880	N	GLU	403	-2.090	10.043	29.529	1.00	23.54
ATOM	1881	CA	GLU	403	-3				

ATOM	1883	CG	GLU	403	-5.469	8.531	28.506	1.00	63.22
ATOM	1884	CD	GLU	403	-6.530	8.952	27.498	1.00	63.22
ATOM	1885	OE1	GLU	403	-6.237	9.786	26.613	1.00	63.22
ATOM	1886	OE2	GLU	403	-7.666	8.436	27.589	1.00	63.22
ATOM	1887	C	GLU	403	-2.708	7.629	29.170	1.00	23.54
ATOM	1888	O	GLU	403	-3.210	6.656	29.735	1.00	63.22
ATOM	1889	N	VAL	404	-1.787	7.515	28.221	1.00	33.24
ATOM	1890	CA	VAL	404	-1.297	6.213	27.782	1.00	33.24
ATOM	1891	CB	VAL	404	-0.621	6.314	26.390	1.00	30.71
ATOM	1892	CG1	VAL	404	-0.097	4.957	25.947	1.00	30.71
ATOM	1893	CG2	VAL	404	-1.611	6.841	25.371	1.00	30.71
ATOM	1894	C	VAL	404	-0.338	5.528	28.752	1.00	33.24
ATOM	1895	O	VAL	404	-0.386	4.305	28.914	1.00	30.71
ATOM	1896	N	PHE	405	0.526	6.309	29.392	1.00	33.66
ATOM	1897	CA	PHE	405	1.516	5.752	30.308	1.00	33.66
ATOM	1898	CB	PHE	405	2.901	6.326	29.984	1.00	34.35
ATOM	1899	CG	PHE	405	3.343	6.076	28.568	1.00	34.35
ATOM	1900	CD1	PHE	405	3.519	7.134	27.683	1.00	34.35
ATOM	1901	CD2	PHE	405	3.569	4.782	28.114	1.00	34.35
ATOM	1902	CE1	PHE	405	3.911	6.906	26.365	1.00	34.35
ATOM	1903	CE2	PHE	405	3.960	4.545	26.798	1.00	34.35
ATOM	1904	CZ	PHE	405	4.131	5.610	25.922	1.00	34.35
ATOM	1905	C	PHE	405	1.189	5.931	31.790	1.00	33.66
ATOM	1906	O	PHE	405	2.036	5.539	32.623	1.00	34.35
ATOM	1907	OXT	PHE	405	0.090	6.434	32.107	1.00	34.35
ATOM	1908	C1	TRI	1	8.375	7.063	18.475	1.00	34.21
ATOM	1909	C2	TRI	1	10.048	8.688	23.016	1.00	33.36
ATOM	1910	C3	TRI	1	8.104	8.391	18.941	1.00	34.21
ATOM	1911	C4	TRI	1	10.496	9.696	23.813	1.00	33.36
ATOM	1912	C5	TRI	1	8.916	8.943	19.927	1.00	34.21
ATOM	1913	C6	TRI	1	10.152	9.772	25.121	1.00	33.36
ATOM	1914	C7	TRI	1	9.862	8.178	20.609	1.00	34.21
ATOM	1915	C8	TRI	1	9.246	8.821	25.653	1.00	33.36
ATOM	1916	C9	TRI	1	10.117	6.865	20.147	1.00	34.21
ATOM	1917	C10	TRI	1	8.805	7.754	24.847	1.00	33.36
ATOM	1918	C11	TRI	1	9.375	6.339	19.026	1.00	34.21
ATOM	1919	C12	TRI	1	9.125	7.756	23.490	1.00	33.36
ATOM	1920	C13	TRI	1	7.540	6.470	17.383	1.00	35.85
ATOM	1921	C15	TRI	1	8.158	6.555	15.938	1.00	35.85
ATOM	1922	I1	TRI	1	8.713	10.990	20.395	1.00	34.21
ATOM	1923	I2	TRI	1	10.951	11.289	26.315	1.00	33.36
ATOM	1924	I3	TRI	1	11.592	5.685	21.118	1.00	34.21
ATOM	1925	O3	TRI	1	9.407	6.654	15.852	1.00	35.85
ATOM	1926	O2	TRI	1	10.570	8.649	21.717	1.00	33.36
ATOM	1927	O1	TRI	1	8.798	8.969	26.979	1.00	33.36
ATOM	1928	O4	TRI	1	7.352	6.522	14.973	1.00	35.85
ATOM	1929	O1							



# APPENDIX 5

## TR\_IPBR2.PDB

REMARK rTR\_ipbr2 full length numbering

REMARK

REMARK Rfactor 0.214 Rfree 0.224

REMARK Resolution 15. 2.2 all reflections

REMARK

REMARK Three cacodylate-modified cysteines (CYA)

REMARK Cya334, Cya380, Cya392

REMARK cacodylate modeled as single arsenic atom

REMARK

REMARK side chain of certain residues modeled as ALA due to poor density;

REMARK however, residue name reflects true residue for clarity

REMARK

REMARK clone obtained from Murray et. al.

REMARK deposited sequence confirmed,

REMARK differing from that reported by Thompson et. al.

REMARK in the following codons:

REMARK 281 Thr - Ala

REMARK 285 Lys - Glu

REMARK identical to that reported by Mitsuhashi et. al.

REMARK gb:RNTRAVI X07409

JRNL AUTH M.B. MURRAY, N.D.ZILZ, N.L.MCCREARY,M.J.MACDONALD

JRNL AUTH 2 H.C.TOWLE

JRNL TITL ISOLATION AND CHARACTERIZATION OF RAT CDNA CLONES  
FOR

TWO

JRNL TITL 2 DISTINCT THYROID HORMONE RECPTORS

JRNL REF JBC V. 263 25 1988

JRNL AUTH C.C.THOMPSON, C.WEINBERGER, R.LEBO, R.M.EVANS

JRNL TITL IDENTIFICATION OF A NOVEL THYROID HORMONE RECEPTOR  
EXPRESSED

JRNL TITL 2 IN THE MAMMALIAN CENTRAL NERVOUS SYSTEM

JRNL REF SCIENCE V. 237 1987

JRNL AUTH T.MITSUHASHI,G.TENNYSON,V.NIKODEM

JRNL TITL NUCLEOTIDE SEQUENCE OF NOVEL CDNAS GENERATED BY  
ALTERNATIVE

JRNL TITL 2 SPLICING OF A RAT THYROID HORMONE RECEPTOR GENE  
TRANSCRIPT

JRNL REF NUC. ACIDS. RES. V. 16 12 1988

REMARK

ATOM 1 CB ARG 157 68.481 10.663 6.906 1.00 57.50

ATOM 2 CG ARG 157 69.793 10.213 7.512 1.00 59.93

ATOM 3 CD ARG 157 70.510 11.365 8.189 1.00 70.24



ATOM	4	NE	ARG	157	71.661	10.906	8.961	1.00	77.62
ATOM	5	CZ	ARG	157	71.599	10.492	10.224	1.00	78.75
ATOM	6	NH1	ARG	157	70.440	10.480	10.870	1.00	74.33
ATOM	7	NH2	ARG	157	72.697	10.075	10.839	1.00	83.44
ATOM	8	C	ARG	157	66.314	10.014	5.809	1.00	46.84
ATOM	9	O	ARG	157	66.109	10.397	4.659	1.00	54.49
ATOM	10	N	ARG	157	68.442	9.069	5.013	1.00	56.54
ATOM	11	CA	ARG	157	67.704	9.537	6.222	1.00	52.92
ATOM	12	N	PRO	158	65.335	9.953	6.727	1.00	39.44
ATOM	13	CD	PRO	158	65.503	9.448	8.099	1.00	41.72
ATOM	14	CA	PRO	158	63.946	10.368	6.487	1.00	34.98
ATOM	15	CB	PRO	158	63.282	10.172	7.854	1.00	34.92
ATOM	16	CG	PRO	158	64.096	9.096	8.487	1.00	45.83
ATOM	17	C	PRO	158	63.765	11.804	5.992	1.00	34.13
ATOM	18	O	PRO	158	64.223	12.757	6.621	1.00	31.07
ATOM	19	N	GLU	159	63.110	11.932	4.841	1.00	31.36
ATOM	20	CA	GLU	159	62.814	13.220	4.228	1.00	27.34
ATOM	21	CB	GLU	159	62.569	13.041	2.726	1.00	24.27
ATOM	22	CG	GLU	159	63.814	12.866	1.887	1.00	24.85
ATOM	23	CD	GLU	159	64.409	14.188	1.454	1.00	28.12
ATOM	24	OE1	GLU	159	63.642	15.144	1.224	1.00	29.26
ATOM	25	OE2	GLU	159	65.646	14.269	1.326	1.00	29.52
ATOM	26	C	GLU	159	61.528	13.707	4.870	1.00	24.30
ATOM	27	O	GLU	159	60.855	12.934	5.566	1.00	29.01
ATOM	28	N	PRO	160	61.192	14.989	4.718	1.00	24.62
ATOM	29	CD	PRO	160	61.979	16.126	4.188	1.00	18.72
ATOM	30	CA	PRO	160	59.947	15.451	5.330	1.00	21.62
ATOM	31	CB	PRO	160	59.945	16.955	5.048	1.00	12.71
ATOM	32	CG	PRO	160	61.394	17.297	4.930	1.00	15.12
ATOM	33	C	PRO	160	58.743	14.752	4.671	1.00	24.61
ATOM	34	O	PRO	160	58.789	14.384	3.490	1.00	22.63
ATOM	35	N	THR	161	57.705	14.504	5.450	1.00	25.86
ATOM	36	CA	THR	161	56.515	13.864	4.921	1.00	23.77
ATOM	37	CB	THR	161	55.689	13.201	6.048	1.00	21.75
ATOM	38	OG1	THR	161	55.178	14.210	6.926	1.00	20.78
ATOM	39	CG2	THR	161	56.549	12.227	6.847	1.00	18.44
ATOM	40	C	THR	161	55.680	14.967	4.269	1.00	28.67
ATOM	41	O	THR	161	55.917	16.151	4.510	1.00	29.90
ATOM	42	N	PRO	162	54.685	14.597	3.448	1.00	27.79
ATOM	43	CD	PRO	162	54.313	13.237	3.019	1.00	23.25
ATOM	44	CA	PRO	162	53.843	15.603	2.795	1.00	26.19
ATOM	45	CB	PRO	162	52.699	14.766	2.227	1.00	19.89
ATOM	46	CG	PRO	162	53.394	13.492	1.848	1.00	20.63
ATOM	47	C	PRO	162	53.334	16.661	3.775	1.00	24.81
ATOM	48	O	PRO	162	53.477	17.863	3.526	1.00	21.10
ATOM	49	N	GLU	163	52.812	16.198	4.911	1.00	26.34
ATOM	50	CA	GLU	163	52.266	17.065			

ATOM	51	CB	GLU	163	51.640	16.231	7.086	1.00	29.46
ATOM	52	CG	GLU	163	50.482	15.321	6.666	1.00	48.37
ATOM	53	CD	GLU	163	50.918	14.132	5.816	1.00	53.12
ATOM	54	OE1	GLU	163	51.890	13.441	6.194	1.00	52.22
ATOM	55	OE2	GLU	163	50.282	13.886	4.766	1.00	59.14
ATOM	56	C	GLU	163	53.353	17.949	6.552	1.00	26.74
ATOM	57	O	GLU	163	53.109	19.107	6.898	1.00	27.03
ATOM	58	N	GLU	164	54.553	17.389	6.677	1.00	26.74
ATOM	59	CA	GLU	164	55.679	18.124	7.221	1.00	23.65
ATOM	60	CB	GLU	164	56.805	17.174	7.609	1.00	18.85
ATOM	61	CG	GLU	164	56.441	16.306	8.804	1.00	26.81
ATOM	62	CD	GLU	164	57.536	15.334	9.188	1.00	31.06
ATOM	63	OE1	GLU	164	58.404	15.050	8.340	1.00	29.21
ATOM	64	OE2	GLU	164	57.524	14.848	10.340	1.00	31.39
ATOM	65	C	GLU	164	56.165	19.204	6.276	1.00	26.54
ATOM	66	O	GLU	164	56.609	20.258	6.724	1.00	32.48
ATOM	67	N	TRP	165	56.075	18.957	4.971	1.00	23.41
ATOM	68	CA	TRP	165	56.488	19.962	3.998	1.00	20.81
ATOM	69	CB	TRP	165	56.462	19.405	2.573	1.00	18.15
ATOM	70	CG	TRP	165	57.762	18.747	2.164	1.00	15.80
ATOM	71	CD2	TRP	165	59.058	19.377	2.064	1.00	15.35
ATOM	72	CE2	TRP	165	59.959	18.392	1.628	1.00	12.14
ATOM	73	CE3	TRP	165	59.527	20.676	2.287	1.00	17.56
ATOM	74	CD1	TRP	165	57.939	17.449	1.804	1.00	12.78
ATOM	75	NE1	TRP	165	59.253	17.230	1.484	1.00	16.10
ATOM	76	CZ2	TRP	165	61.318	18.657	1.419	1.00	16.26
ATOM	77	CZ3	TRP	165	60.879	20.944	2.079	1.00	19.52
ATOM	78	CH2	TRP	165	61.760	19.933	1.642	1.00	16.48
ATOM	79	C	TRP	165	55.547	21.151	4.109	1.00	19.66
ATOM	80	O	TRP	165	55.975	22.295	3.960	1.00	23.61
ATOM	81	N	ASP	166	54.269	20.882	4.376	1.00	22.66
ATOM	82	CA	ASP	166	53.269	21.943	4.537	1.00	23.35
ATOM	83	CB	ASP	166	51.863	21.359	4.716	1.00	22.61
ATOM	84	CG	ASP	166	51.347	20.681	3.458	1.00	31.41
ATOM	85	OD1	ASP	166	51.816	21.028	2.360	1.00	26.38
ATOM	86	OD2	ASP	166	50.464	19.803	3.570	1.00	32.25
ATOM	87	C	ASP	166	53.631	22.760	5.773	1.00	26.47
ATOM	88	O	ASP	166	53.694	23.991	5.718	1.00	30.25
ATOM	89	N	LEU	167	53.887	22.054	6.872	1.00	24.12
ATOM	90	CA	LEU	167	54.268	22.663	8.139	1.00	26.44
ATOM	91	CB	LEU	167	54.596	21.557	9.148	1.00	32.57
ATOM	92	CG	LEU	167	54.659	21.919	10.629	1.00	36.97
ATOM	93	CD1	LEU	167	53.289	22.402	11.080	1.00	43.83
ATOM	94	CD2	LEU	167	55.096	20.712	11.448	1.00	34.75
ATOM	95	C	LEU	167	55.501	23.533	7.904	1.00	23.19
ATOM	96	O	LEU	167	55.570	24.670	8.368	1.00	28.18

ATOM	98	CA	ILE	168	57.703	23.651	6.801	1.00	17.71
ATOM	99	CB	ILE	168	58.632	22.693	6.006	1.00	14.43
ATOM	100	CG2	ILE	168	59.740	23.451	5.304	1.00	16.71
ATOM	101	CG1	ILE	168	59.219	21.644	6.948	1.00	21.24
ATOM	102	CD1	ILE	168	60.063	20.588	6.264	1.00	18.18
ATOM	103	C -	ILE	168	57.475	24.931	6.002	1.00	28.73
ATOM	104	O	ILE	168	58.064	25.977	6.307	1.00	29.36
ATOM	105	N	HIS	169	56.601	24.866	5.005	1.00	24.43
ATOM	106	CA	HIS	169	56.319	26.027	4.169	1.00	23.64
ATOM	107	CB	HIS	169	55.459	25.631	2.971	1.00	23.55
ATOM	108	CG	HIS	169	56.140	24.683	2.034	1.00	23.82
ATOM	109	CD2	HIS	169	57.455	24.429	1.824	1.00	19.23
ATOM	110	ND1	HIS	169	55.450	23.833	1.199	1.00	22.92
ATOM	111	CE1	HIS	169	56.302	23.089	0.522	1.00	19.56
ATOM	112	NE2	HIS	169	57.527	23.431	0.883	1.00	26.00
ATOM	113	C	HIS	169	55.653	27.135	4.962	1.00	19.37
ATOM	114	O	HIS	169	56.069	28.288	4.880	1.00	25.64
ATOM	115	N	VAL	170	54.638	26.782	5.745	1.00	19.88
ATOM	116	CA	VAL	170	53.925	27.758	6.555	1.00	20.28
ATOM	117	CB	VAL	170	52.755	27.100	7.330	1.00	26.06
ATOM	118	CG1	VAL	170	52.093	28.109	8.259	1.00	20.15
ATOM	119	CG2	VAL	170	51.725	26.541	6.352	1.00	18.69
ATOM	120	C	VAL	170	54.886	28.442	7.532	1.00	23.11
ATOM	121	O	VAL	170	54.907	29.672	7.625	1.00	28.86
ATOM	122	N	ALA	171	55.716	27.644	8.203	1.00	20.48
ATOM	123	CA	ALA	171	56.686	28.146	9.173	1.00	19.84
ATOM	124	CB	ALA	171	57.365	26.985	9.902	1.00	18.07
ATOM	125	C	ALA	171	57.728	29.049	8.512	1.00	20.62
ATOM	126	O	ALA	171	58.033	30.127	9.037	1.00	24.67
ATOM	127	N	THR	172	58.251	28.632	7.359	1.00	20.65
ATOM	128	CA	THR	172	59.247	29.428	6.640	1.00	18.91
ATOM	129	CB	THR	172	59.755	28.709	5.380	1.00	20.06
ATOM	130	OG1	THR	172	60.267	27.417	5.734	1.00	20.30
ATOM	131	CG2	THR	172	60.877	29.516	4.726	1.00	18.38
ATOM	132	C	THR	172	58.675	30.786	6.235	1.00	24.43
ATOM	133	O	THR	172	59.346	31.815	6.360	1.00	23.54
ATOM	134	N	GLU	173	57.430	30.792	5.766	1.00	24.33
ATOM	135	CA	GLU	173	56.783	32.031	5.361	1.00	25.98
ATOM	136	CB	GLU	173	55.460	31.734	4.651	1.00	28.39
ATOM	137	CG	GLU	173	54.679	32.974	4.207	1.00	40.39
ATOM	138	CD	GLU	173	55.487	33.951	3.347	1.00	48.33
ATOM	139	OE1	GLU	173	55.261	35.172	3.478	1.00	51.86
ATOM	140	OE2	GLU	173	56.334	33.513	2.533	1.00	46.92
ATOM	141	C	GLU	173	56.564	32.953	6.562	1.00	25.57
ATOM	142	O	GLU	173	56.877	34.141	6.498	1.00	27.76
ATOM	143	N	ALA	174	56.071	32.383	7.664	1.00	25.31





ATOM	192	CB	ALA	180	63.653	43.390	10.346	1.00	29.96
ATOM	193	C	ALA	180	64.481	42.481	8.182	1.00	37.02
ATOM	194	O	ALA	180	65.518	41.866	8.414	1.00	41.85
ATOM	195	N	GLN	181	64.266	43.163	7.057	1.00	37.15
ATOM	196	CA	GLN	181	65.261	43.306	5.995	1.00	39.33
ATOM	197	CB	GLN	181	66.572	43.877	6.552	1.00	37.42
ATOM	198	CG	GLN	181	66.420	45.190	7.309	1.00	44.86
ATOM	199	CD	GLN	181	65.779	46.285	6.479	1.00	53.60
ATOM	200	OE1	GLN	181	64.712	46.793	6.821	1.00	58.51
ATOM	201	NE2	GLN	181	66.422	46.650	5.378	1.00	63.36
ATOM	202	C	GLN	181	65.549	42.053	5.164	1.00	44.18
ATOM	203	O	GLN	181	66.367	42.102	4.239	1.00	46.35
ATOM	204	N	GLY	182	64.873	40.949	5.474	1.00	43.76
ATOM	205	CA	GLY	182	65.074	39.713	4.732	1.00	46.26
ATOM	206	C	GLY	182	66.531	39.363	4.477	1.00	49.98
ATOM	207	O	GLY	182	67.309	39.175	5.419	1.00	56.26
ATOM	208	N	SER	183	66.907	39.274	3.205	1.00	50.96
ATOM	209	CA	SER	183	68.281	38.947	2.830	1.00	55.69
ATOM	210	CB	SER	183	68.284	38.024	1.608	1.00	56.52
ATOM	211	OG	SER	183	67.398	38.497	0.609	1.00	60.82
ATOM	212	C	SER	183	69.121	40.197	2.558	1.00	59.84
ATOM	213	O	SER	183	70.352	40.138	2.540	1.00	66.02
ATOM	214	N	HIS	184	68.453	41.338	2.413	1.00	60.68
ATOM	215	CA	HIS	184	69.131	42.600	2.139	1.00	60.01
ATOM	216	CB	HIS	184	68.150	43.596	1.517	1.00	53.49
ATOM	217	C	HIS	184	69.798	43.209	3.380	1.00	59.43
ATOM	218	O	HIS	184	70.373	44.300	3.303	1.00	59.56
ATOM	219	N	TRP	185	69.753	42.500	4.508	1.00	57.54
ATOM	220	CA	TRP	185	70.343	42.995	5.754	1.00	54.25
ATOM	221	CB	TRP	185	70.147	41.988	6.899	1.00	47.54
ATOM	222	CG	TRP	185	70.905	40.692	6.752	1.00	41.08
ATOM	223	CD2	TRP	185	72.233	40.404	7.230	1.00	39.59
ATOM	224	CE2	TRP	185	72.522	39.070	6.874	1.00	30.27
ATOM	225	CE3	TRP	185	73.202	41.146	7.919	1.00	35.23
ATOM	226	CD1	TRP	185	70.462	39.553	6.149	1.00	39.73
ATOM	227	NE1	TRP	185	71.427	38.577	6.219	1.00	40.01
ATOM	228	CZ2	TRP	185	73.740	38.457	7.188	1.00	31.35
ATOM	229	CZ3	TRP	185	74.416	40.535	8.230	1.00	32.76
ATOM	230	CH2	TRP	185	74.673	39.203	7.861	1.00	31.71
ATOM	231	C	TRP	185	71.818	43.382	5.655	1.00	54.21
ATOM	232	O	TRP	185	72.229	44.403	6.200	1.00	52.82
ATOM	233	N	LYS	186	72.605	42.584	4.938	1.00	54.57
ATOM	234	CA	LYS	186	74.034	42.848	4.788	1.00	55.46
ATOM	235	CB	LYS	186	74.712	41.682	4.080	1.00	53.31
ATOM	236	C	LYS	186	74.338	44.160	4.061	1.00	58.96
ATOM	237	O	LYS	186	75.417	44.731	4.226</		



ATOM	239	CA	GLN	187	73.563	45.873	2.512	1.00	60.15
ATOM	240	CB	GLN	187	73.157	45.653	1.050	1.00	57.00
ATOM	241	C	GLN	187	72.809	47.064	3.101	1.00	60.91
ATOM	242	O	GLN	187	73.149	48.213	2.822	1.00	66.50
ATOM	243	N	ARG	188	71.795	46.790	3.919	1.00	59.55
ATOM	244	CA	ARG	188	70.983	47.847	4.525	1.00	59.26
ATOM	245	CB	ARG	188	69.504	47.462	4.466	1.00	55.21
ATOM	246	C	ARG	188	71.372	48.243	5.959	1.00	58.97
ATOM	247	O	ARG	188	70.914	49.269	6.469	1.00	58.54
ATOM	248	N	ARG	189	72.202	47.432	6.607	1.00	55.46
ATOM	249	CA	ARG	189	72.630	47.704	7.979	1.00	52.98
ATOM	250	CB	ARG	189	73.211	46.437	8.619	1.00	47.73
ATOM	251	CG	ARG	189	74.509	45.985	7.989	1.00	47.88
ATOM	252	CD	ARG	189	75.080	44.763	8.654	1.00	46.96
ATOM	253	NE	ARG	189	76.377	44.441	8.068	1.00	57.93
ATOM	254	CZ	ARG	189	77.450	44.090	8.768	1.00	64.81
ATOM	255	NH1	ARG	189	77.385	44.005	10.087	1.00	67.27
ATOM	256	NH2	ARG	189	78.600	43.860	8.148	1.00	67.84
ATOM	257	C	ARG	189	73.650	48.838	8.091	1.00	53.48
ATOM	258	O	ARG	189	74.513	49.004	7.227	1.00	57.14
ATOM	259	N	LYS	190	73.533	49.617	9.161	1.00	51.31
ATOM	260	CA	LYS	190	74.444	50.722	9.435	1.00	48.83
ATOM	261	CB	LYS	190	73.682	52.036	9.516	1.00	45.36
ATOM	262	C	LYS	190	75.101	50.411	10.773	1.00	46.88
ATOM	263	O	LYS	190	74.454	49.872	11.675	1.00	48.81
ATOM	264	N	PHE	191	76.385	50.724	10.894	1.00	46.98
ATOM	265	CA	PHE	191	77.123	50.462	12.125	1.00	44.38
ATOM	266	CB	PHE	191	78.630	50.520	11.873	1.00	44.25
ATOM	267	CG	PHE	191	79.170	49.336	11.123	1.00	49.51
ATOM	268	CD1	PHE	191	78.828	49.124	9.791	1.00	52.20
ATOM	269	CD2	PHE	191	80.029	48.437	11.748	1.00	47.25
ATOM	270	CE1	PHE	191	79.335	48.031	9.090	1.00	55.86
ATOM	271	CE2	PHE	191	80.542	47.343	11.059	1.00	49.73
ATOM	272	CZ	PHE	191	80.195	47.139	9.727	1.00	51.55
ATOM	273	C	PHE	191	76.764	51.443	13.233	1.00	46.44
ATOM	274	O	PHE	191	76.647	52.645	12.996	1.00	51.28
ATOM	275	N	LEU	192	76.567	50.924	14.439	1.00	47.66
ATOM	276	CA	LEU	192	76.256	51.776	15.577	1.00	46.44
ATOM	277	CB	LEU	192	75.930	50.924	16.808	1.00	38.06
ATOM	278	CG	LEU	192	75.527	51.672	18.082	1.00	33.55
ATOM	279	CD1	LEU	192	74.180	52.339	17.871	1.00	28.17
ATOM	280	CD2	LEU	192	75.476	50.717	19.268	1.00	26.95
ATOM	281	C	LEU	192	77.524	52.595	15.824	1.00	45.82
ATOM	282	O	LEU	192	78.604	52.024	16.008	1.00	41.65
ATOM	283	N	PRO	193	77.422	53.936	15.782	1.00	48.88
ATOM	284	CD	PRO	193	76.176	54.701	15		

ATOM	286	CB	PRO	193	77.879	56.162	16.319	1.00	46.04
ATOM	287	CG	PRO	193	76.675	56.126	15.438	1.00	46.24
ATOM	288	C	PRO	193	79.475	54.377	17.137	1.00	49.60
ATOM	289	O	PRO	193	79.000	54.033	18.218	1.00	54.05
ATOM	290	N	ASP	194	80.783	54.383	16.891	1.00	50.63
ATOM	291	CA	ASP	194	81.769	53.951	17.885	1.00	54.57
ATOM	292	CB	ASP	194	83.164	53.965	17.272	1.00	59.28
ATOM	293	CG	ASP	194	83.309	52.952	16.170	1.00	66.39
ATOM	294	OD1	ASP	194	83.057	53.311	14.998	1.00	72.95
ATOM	295	OD2	ASP	194	83.640	51.787	16.486	1.00	69.00
ATOM	296	C	ASP	194	81.769	54.726	19.198	1.00	54.41
ATOM	297	O	ASP	194	82.229	54.221	20.222	1.00	55.27
ATOM	298	N	ASP	195	81.268	55.956	19.168	1.00	57.20
ATOM	299	CA	ASP	195	81.206	56.775	20.371	1.00	59.68
ATOM	300	CB	ASP	195	81.017	58.261	20.006	1.00	62.99
ATOM	301	CG	ASP	195	79.747	58.526	19.187	1.00	71.67
ATOM	302	OD1	ASP	195	78.734	58.956	19.796	1.00	70.17
ATOM	303	OD2	ASP	195	79.782	58.311	17.951	1.00	75.23
ATOM	304	C	ASP	195	80.092	56.289	21.306	1.00	58.39
ATOM	305	O	ASP	195	80.032	56.676	22.474	1.00	59.81
ATOM	306	N	ILE	196	79.245	55.399	20.794	1.00	54.47
ATOM	307	CA	ILE	196	78.141	54.840	21.568	1.00	49.00
ATOM	308	CB	ILE	196	76.839	54.780	20.731	1.00	46.64
ATOM	309	CG2	ILE	196	75.701	54.195	21.560	1.00	42.11
ATOM	310	CG1	ILE	196	76.467	56.184	20.241	1.00	44.23
ATOM	311	CD1	ILE	196	75.214	56.238	19.373	1.00	48.45
ATOM	312	C	ILE	196	78.497	53.436	22.068	1.00	46.22
ATOM	313	O	ILE	196	78.912	52.570	21.298	1.00	42.07
ATOM	314	N	GLY	197	78.357	53.228	23.370	1.00	45.62
ATOM	315	CA	GLY	197	78.658	51.930	23.941	1.00	51.49
ATOM	316	C	GLY	197	80.005	51.832	24.625	1.00	54.64
ATOM	317	O	GLY	197	80.377	50.759	25.092	1.00	49.98
ATOM	318	N	GLN	198	80.726	52.946	24.725	1.00	60.08
ATOM	319	CA	GLN	198	82.039	52.939	25.366	1.00	61.01
ATOM	320	CB	GLN	198	83.082	53.568	24.441	1.00	55.55
ATOM	321	C	GLN	198	82.044	53.633	26.733	1.00	59.57
ATOM	322	O	GLN	198	83.103	54.016	27.232	1.00	61.30
ATOM	323	N	SER	199	80.875	53.738	27.362	1.00	57.27
ATOM	324	CA	SER	199	80.758	54.397	28.665	1.00	50.61
ATOM	325	CB	SER	199	80.276	55.842	28.478	1.00	53.70
ATOM	326	OG	SER	199	81.010	56.508	27.463	1.00	61.92
ATOM	327	C	SER	199	79.848	53.684	29.675	1.00	46.41
ATOM	328	O	SER	199	78.798	54.210	30.060	1.00	41.16
ATOM	329	N	PRO	200	80.222	52.466	30.096	1.00	42.08
ATOM	330	CD	PRO	200	81.349	51.648	29.605	1.00	38.31
ATOM	331	CA	PRO	200	79.409				

ATOM	333	CG	PRO	200	81.377	50.504	30.583	1.00	37.43
ATOM	334	C	PRO	200	79.615	52.270	32.485	1.00	50.91
ATOM	335	O	PRO	200	80.629	51.980	33.123	1.00	55.65
ATOM	336	N	ILE	201	78.663	53.060	32.975	1.00	55.81
ATOM	337	CA	ILE	201	78.781	53.651	34.311	1.00	57.24
ATOM	338	CB	ILE	201	78.861	55.192	34.250	1.00	58.40
ATOM	339	CG2	ILE	201	80.218	55.622	33.709	1.00	60.49
ATOM	340	CG1	ILE	201	77.716	55.751	33.404	1.00	62.42
ATOM	341	CD1	ILE	201	77.819	57.234	33.137	1.00	61.68
ATOM	342	C	ILE	201	77.728	53.241	35.332	1.00	56.52
ATOM	343	O	ILE	201	77.961	53.352	36.537	1.00	60.89
ATOM	344	N	VAL	202	76.564	52.794	34.871	1.00	52.76
ATOM	345	CA	VAL	202	75.522	52.366	35.802	1.00	47.37
ATOM	346	CB	VAL	202	74.117	52.377	35.153	1.00	38.14
ATOM	347	CG1	VAL	202	73.092	51.804	36.117	1.00	30.35
ATOM	348	CG2	VAL	202	73.730	53.798	34.763	1.00	26.69
ATOM	349	C	VAL	202	75.885	50.958	36.285	1.00	53.65
ATOM	350	O	VAL	202	75.914	50.010	35.500	1.00	55.10
ATOM	351	N	SER	203	76.226	50.839	37.561	1.00	59.85
ATOM	352	CA	SER	203	76.614	49.556	38.132	1.00	64.58
ATOM	353	CB	SER	203	77.209	49.749	39.532	1.00	68.95
ATOM	354	OG	SER	203	78.396	50.523	39.483	1.00	74.02
ATOM	355	C	SER	203	75.493	48.528	38.197	1.00	61.69
ATOM	356	O	SER	203	74.351	48.846	38.535	1.00	63.63
ATOM	357	N	MET	204	75.848	47.295	37.859	1.00	57.37
ATOM	358	CA	MET	204	74.932	46.162	37.885	1.00	57.54
ATOM	359	CB	MET	204	74.847	45.505	36.501	1.00	56.59
ATOM	360	CG	MET	204	74.012	46.270	35.489	1.00	44.08
ATOM	361	SD	MET	204	72.255	46.228	35.884	1.00	46.62
ATOM	362	CE	MET	204	71.775	44.758	35.013	1.00	48.37
ATOM	363	C	MET	204	75.522	45.178	38.888	1.00	55.86
ATOM	364	O	MET	204	76.746	45.089	39.027	1.00	58.94
ATOM	365	N	PRO	205	74.671	44.432	39.607	1.00	55.36
ATOM	366	CD	PRO	205	73.203	44.570	39.625	1.00	57.73
ATOM	367	CA	PRO	205	75.119	43.453	40.604	1.00	56.82
ATOM	368	CB	PRO	205	73.814	43.042	41.295	1.00	59.79
ATOM	369	CG	PRO	205	72.769	43.281	40.255	1.00	57.85
ATOM	370	C	PRO	205	75.902	42.239	40.083	1.00	57.25
ATOM	371	O	PRO	205	75.683	41.118	40.541	1.00	66.28
ATOM	372	N	ASP	206	76.822	42.462	39.147	1.00	58.75
ATOM	373	CA	ASP	206	77.639	41.389	38.586	1.00	61.09
ATOM	374	CB	ASP	206	76.802	40.462	37.685	1.00	66.07
ATOM	375	CG	ASP	206	76.158	41.190	36.521	1.00	70.97
ATOM	376	OD1	ASP	206	74.989	41.613	36.662	1.00	76.97
ATOM	377	OD2	ASP	206	76.813	41.322	35.465	1.00	61.12
ATOM	378	C	ASP	206	78.865	41.910</			

ATOM	380	N	GLY	207	79.282	43.130	38.158	1.00	63.00
ATOM	381	CA	GLY	207	80.455	43.709	37.522	1.00	64.43
ATOM	382	C	GLY	207	80.224	44.467	36.229	1.00	64.81
ATOM	383	O	GLY	207	80.649	45.619	36.110	1.00	68.76
ATOM	384	N	ASP	208	79.584	43.827	35.253	1.00	63.53
ATOM	385	CA	ASP	208	79.316	44.459	33.962	1.00	58.96
ATOM	386	CB	ASP	208	78.746	43.434	32.974	1.00	62.84
ATOM	387	CG	ASP	208	79.743	42.336	32.633	1.00	64.73
ATOM	388	OD1	ASP	208	79.575	41.200	33.121	1.00	66.65
ATOM	389	OD2	ASP	208	80.701	42.610	31.878	1.00	68.91
ATOM	390	C	ASP	208	78.368	45.646	34.110	1.00	56.65
ATOM	391	O	ASP	208	77.182	45.473	34.392	1.00	55.79
ATOM	392	N	LYS	209	78.911	46.852	33.953	1.00	54.66
ATOM	393	CA	LYS	209	78.132	48.081	34.082	1.00	53.92
ATOM	394	CB	LYS	209	79.034	49.236	34.515	1.00	49.71
ATOM	395	C	LYS	209	77.395	48.420	32.785	1.00	48.30
ATOM	396	O	LYS	209	77.767	47.945	31.711	1.00	45.62
ATOM	397	N	VAL	210	76.367	49.258	32.894	1.00	43.87
ATOM	398	CA	VAL	210	75.539	49.662	31.757	1.00	41.25
ATOM	399	CB	VAL	210	74.020	49.624	32.125	1.00	32.99
ATOM	400	CG1	VAL	210	73.153	50.029	30.937	1.00	31.44
ATOM	401	CG2	VAL	210	73.626	48.239	32.604	1.00	27.57
ATOM	402	C	VAL	210	75.868	51.061	31.234	1.00	43.30
ATOM	403	O	VAL	210	76.261	51.951	31.994	1.00	44.65
ATOM	404	N	ASP	211	75.688	51.235	29.931	1.00	43.23
ATOM	405	CA	ASP	211	75.906	52.498	29.240	1.00	40.62
ATOM	406	CB	ASP	211	76.686	52.232	27.943	1.00	43.49
ATOM	407	CG	ASP	211	77.014	53.499	27.161	1.00	40.77
ATOM	408	OD1	ASP	211	76.180	54.427	27.092	1.00	42.13
ATOM	409	OD2	ASP	211	78.111	53.549	26.574	1.00	37.49
ATOM	410	C	ASP	211	74.491	53.001	28.921	1.00	44.56
ATOM	411	O	ASP	211	73.849	52.500	27.998	1.00	46.44
ATOM	412	N	LEU	212	74.006	53.982	29.684	1.00	43.76
ATOM	413	CA	LEU	212	72.662	54.538	29.494	1.00	41.47
ATOM	414	CB	LEU	212	72.473	55.785	30.359	1.00	40.45
ATOM	415	CG	LEU	212	72.360	55.585	31.867	1.00	44.47
ATOM	416	CD1	LEU	212	72.127	56.923	32.551	1.00	40.49
ATOM	417	CD2	LEU	212	71.217	54.634	32.153	1.00	45.94
ATOM	418	C	LEU	212	72.325	54.886	28.049	1.00	40.77
ATOM	419	O	LEU	212	71.254	54.540	27.548	1.00	42.25
ATOM	420	N	GLU	213	73.241	55.588	27.394	1.00	42.53
ATOM	421	CA	GLU	213	73.068	56.008	26.009	1.00	43.60
ATOM	422	CB	GLU	213	74.267	56.860	25.598	1.00	43.84
ATOM	423	CG	GLU	213	74.246	57.334	24.167	1.00	51.70
ATOM	424	CD	GLU	213	75.598	57.848	23.722	1.00	59.23
ATOM	425	OE1	GLU	2					



ATOM	427	C	GLU	213	72.913	54.810	25.066	1.00	42.63
ATOM	428	O	GLU	213	72.008	54.779	24.226	1.00	37.04
ATOM	429	N	ALA	214	73.775	53.814	25.245	1.00	39.28
ATOM	430	CA	ALA	214	73.753	52.605	24.424	1.00	39.52
ATOM	431	CB	ALA	214	74.952	51.726	24.740	1.00	35.16
ATOM	432	C	ALA	214	72.460	51.852	24.694	1.00	37.14
ATOM	433	O	ALA	214	71.795	51.390	23.767	1.00	42.29
ATOM	434	N	PHE	215	72.098	51.773	25.970	1.00	31.60
ATOM	435	CA	PHE	215	70.883	51.102	26.404	1.00	31.67
ATOM	436	CB	PHE	215	70.728	51.217	27.922	1.00	24.80
ATOM	437	CG	PHE	215	69.512	50.522	28.458	1.00	21.78
ATOM	438	CD1	PHE	215	69.553	49.171	28.771	1.00	24.64
ATOM	439	CD2	PHE	215	68.328	51.223	28.658	1.00	21.53
ATOM	440	CE1	PHE	215	68.429	48.528	29.277	1.00	27.63
ATOM	441	CE2	PHE	215	67.200	50.591	29.163	1.00	21.60
ATOM	442	CZ	PHE	215	67.249	49.242	29.472	1.00	21.35
ATOM	443	C	PHE	215	69.675	51.706	25.694	1.00	35.75
ATOM	444	O	PHE	215	68.838	50.975	25.161	1.00	34.84
ATOM	445	N	SER	216	69.604	53.035	25.665	1.00	39.09
ATOM	446	CA	SER	216	68.506	53.739	25.001	1.00	40.61
ATOM	447	CB	SER	216	68.668	55.249	25.165	1.00	43.86
ATOM	448	OG	SER	216	68.616	55.603	26.537	1.00	68.66
ATOM	449	C	SER	216	68.444	53.380	23.518	1.00	40.76
ATOM	450	O	SER	216	67.362	53.161	22.969	1.00	35.50
ATOM	451	N	GLU	217	69.611	53.332	22.878	1.00	38.37
ATOM	452	CA	GLU	217	69.709	52.989	21.462	1.00	37.80
ATOM	453	CB	GLU	217	71.164	53.049	20.997	1.00	39.67
ATOM	454	CG	GLU	217	71.701	54.461	20.880	1.00	46.65
ATOM	455	CD	GLU	217	70.881	55.315	19.925	1.00	53.25
ATOM	456	OE1	GLU	217	70.920	55.056	18.702	1.00	57.12
ATOM	457	OE2	GLU	217	70.189	56.240	20.400	1.00	54.13
ATOM	458	C	GLU	217	69.135	51.598	21.209	1.00	38.48
ATOM	459	O	GLU	217	68.416	51.378	20.228	1.00	43.00
ATOM	460	N	PHE	218	69.426	50.677	22.120	1.00	35.49
ATOM	461	CA	PHE	218	68.934	49.313	22.018	1.00	31.76
ATOM	462	CB	PHE	218	69.743	48.392	22.925	1.00	29.10
ATOM	463	CG	PHE	218	71.169	48.260	22.510	1.00	26.25
ATOM	464	CD1	PHE	218	72.176	48.177	23.459	1.00	24.59
ATOM	465	CD2	PHE	218	71.510	48.233	21.163	1.00	23.53
ATOM	466	CE1	PHE	218	73.504	48.072	23.073	1.00	27.68
ATOM	467	CE2	PHE	218	72.832	48.128	20.765	1.00	25.37
ATOM	468	CZ	PHE	218	73.834	48.047	21.721	1.00	28.43
ATOM	469	C	PHE	218	67.445	49.202	22.321	1.00	31.30
ATOM	470	O	PHE	218	66.726	48.496	21.621	1.00	35.18
ATOM	471	N	THR	219	66.967	49.915	23.333	1.00	30.54
ATOM	472	CA	THR	219	65.				



ATOM	474	OG1 THR	219	65.903	51.746	25.157	1.00	42.99
ATOM	475	CG2 THR	219	65.797	49.562	26.145	1.00	34.32
ATOM	476	C THR	219	64.680	50.514	22.609	1.00	34.53
ATOM	477	O THR	219	63.507	50.162	22.450	1.00	36.57
ATOM	478	N LYS	220	65.267	51.457	21.873	1.00	38.13
ATOM	479	CA LYS	220	64.563	52.158	20.806	1.00	41.42
ATOM	480	CB LYS	220	65.452	53.257	20.208	1.00	41.62
ATOM	481	C LYS	220	64.140	51.182	19.716	1.00	41.80
ATOM	482	O LYS	220	63.032	51.274	19.192	1.00	43.29
ATOM	483	N ILE	221	65.018	50.234	19.393	1.00	36.93
ATOM	484	CA ILE	221	64.726	49.250	18.355	1.00	37.33
ATOM	485	CB ILE	221	65.965	48.932	17.482	1.00	33.71
ATOM	486	CG2 ILE	221	66.491	50.202	16.826	1.00	41.26
ATOM	487	CG1 ILE	221	67.042	48.235	18.309	1.00	30.36
ATOM	488	CD1 ILE	221	68.178	47.687	17.472	1.00	26.28
ATOM	489	C ILE	221	64.141	47.922	18.845	1.00	40.49
ATOM	490	O ILE	221	63.593	47.159	18.048	1.00	43.43
ATOM	491	N ILE	222	64.219	47.651	20.144	1.00	39.43
ATOM	492	CA ILE	222	63.703	46.394	20.667	1.00	35.49
ATOM	493	CB ILE	222	64.169	46.133	22.130	1.00	34.06
ATOM	494	CG2 ILE	222	63.287	46.881	23.130	1.00	26.15
ATOM	495	CG1 ILE	222	64.155	44.627	22.405	1.00	34.08
ATOM	496	CD1 ILE	222	64.760	44.220	23.719	1.00	33.67
ATOM	497	C ILE	222	62.186	46.230	20.539	1.00	37.60
ATOM	498	O ILE	222	61.703	45.127	20.279	1.00	42.14
ATOM	499	N THR	223	61.438	47.324	20.665	1.00	34.60
ATOM	500	CA THR	223	59.979	47.257	20.562	1.00	35.96
ATOM	501	CB THR	223	59.323	48.645	20.799	1.00	41.70
ATOM	502	OG1 THR	223	59.681	49.119	22.106	1.00	44.59
ATOM	503	CG2 THR	223	57.796	48.548	20.706	1.00	42.58
ATOM	504	C THR	223	59.478	46.614	19.252	1.00	34.77
ATOM	505	O THR	223	58.671	45.680	19.289	1.00	30.60
ATOM	506	N PRO	224	59.942	47.103	18.084	1.00	31.99
ATOM	507	CD PRO	224	60.784	48.288	17.839	1.00	30.37
ATOM	508	CA PRO	224	59.496	46.517	16.815	1.00	29.25
ATOM	509	CB PRO	224	60.225	47.366	15.769	1.00	29.27
ATOM	510	CG PRO	224	60.393	48.677	16.441	1.00	36.31
ATOM	511	C PRO	224	59.913	45.050	16.723	1.00	29.20
ATOM	512	O PRO	224	59.146	44.209	16.251	1.00	33.73
ATOM	513	N ALA	225	61.124	44.754	17.192	1.00	19.86
ATOM	514	CA ALA	225	61.663	43.395	17.175	1.00	19.61
ATOM	515	CB ALA	225	63.086	43.388	17.730	1.00	19.08
ATOM	516	C ALA	225	60.777	42.428	17.960	1.00	20.48
ATOM	517	O ALA	225	60.474	41.331	17.489	1.00	24.33
ATOM	518	N ILE	226	60.330	42.847	19.141	1.00	23.72
ATOM	519	CA ILE	226	59.471	42.001	19.972	1.00	21.94
ATOM	520	CB ILE	226	59.152	42.667	21.333	1.00	21.01

ATOM	521	CG2 ILE	226	58.118	41.846	22.095	1.00	15.14
ATOM	522	CG1 ILE	226	60.425	42.841	22.163	1.00	20.45
ATOM	523	CD1 ILE	226	60.216	43.741	23.358	1.00	17.65
ATOM	524	C ILE	226	58.165	41.758	19.228	1.00	24.04
ATOM	525	O ILE	226	57.640	40.642	19.220	1.00	26.92
ATOM	526	N- THR	227	57.653	42.811	18.596	1.00	25.22
ATOM	527	CA THR	227	56.410	42.730	17.836	1.00	27.92
ATOM	528	CB THR	227	55.984	44.132	17.333	1.00	34.33
ATOM	529	OG1 THR	227	55.823	45.007	18.458	1.00	33.62
ATOM	530	CG2 THR	227	54.669	44.061	16.563	1.00	39.18
ATOM	531	C THR	227	56.524	41.733	16.671	1.00	23.61
ATOM	532	O THR	227	55.587	40.977	16.413	1.00	24.41
ATOM	533	N ARG	228	57.670	41.704	15.995	1.00	15.49
ATOM	534	CA ARG	228	57.872	40.773	14.885	1.00	17.92
ATOM	535	CB ARG	228	59.174	41.075	14.137	1.00	19.84
ATOM	536	CG ARG	228	59.203	42.437	13.452	1.00	20.62
ATOM	537	CD ARG	228	60.351	42.523	12.453	1.00	24.29
ATOM	538	NE ARG	228	61.641	42.168	13.047	1.00	27.04
ATOM	539	CZ ARG	228	62.452	43.039	13.642	1.00	37.92
ATOM	540	NH1 ARG	228	62.113	44.327	13.725	1.00	42.82
ATOM	541	NH2 ARG	228	63.618	42.634	14.136	1.00	34.80
ATOM	542	C ARG	228	57.870	39.323	15.387	1.00	22.51
ATOM	543	O ARG	228	57.402	38.421	14.686	1.00	28.49
ATOM	544	N VAL	229	58.362	39.104	16.607	1.00	21.46
ATOM	545	CA VAL	229	58.372	37.762	17.187	1.00	20.12
ATOM	546	CB VAL	229	59.149	37.707	18.524	1.00	17.21
ATOM	547	CG1 VAL	229	59.023	36.322	19.152	1.00	13.73
ATOM	548	CG2 VAL	229	60.611	38.019	18.287	1.00	15.80
ATOM	549	C VAL	229	56.926	37.348	17.421	1.00	19.19
ATOM	550	O VAL	229	56.528	36.224	17.089	1.00	19.86
ATOM	551	N VAL	230	56.134	38.275	17.953	1.00	21.49
ATOM	552	CA VAL	230	54.721	38.023	18.217	1.00	17.69
ATOM	553	CB VAL	230	54.041	39.239	18.881	1.00	21.30
ATOM	554	CG1 VAL	230	52.568	38.952	19.090	1.00	17.26
ATOM	555	CG2 VAL	230	54.706	39.572	20.218	1.00	17.13
ATOM	556	C VAL	230	54.003	37.707	16.902	1.00	26.39
ATOM	557	O VAL	230	53.180	36.790	16.843	1.00	29.63
ATOM	558	N ASP	231	54.333	38.451	15.848	1.00	25.52
ATOM	559	CA ASP	231	53.724	38.242	14.537	1.00	26.78
ATOM	560	CB ASP	231	54.132	39.353	13.571	1.00	23.70
ATOM	561	CG ASP	231	53.649	40.728	14.012	1.00	31.60
ATOM	562	OD1 ASP	231	52.656	40.820	14.771	1.00	31.79
ATOM	563	OD2 ASP	231	54.271	41.727	13.593	1.00	35.74
ATOM	564	C ASP	231	54.108	36.879	13.970	1.00	27.69
ATOM	565	O ASP	231	53.279	36.196	13.366	1.00	25.15
ATOM	566	N PHE	232	55.364	36.490	14.170	1.00	22.29
ATOM	567	CA PHE	232	55.858	35.200	13.703	1.00	23.78

ATOM	568	CB	PHE	232	57.328	35.008	14.097	1.00	24.76
ATOM	569	CG	PHE	232	57.794	33.581	14.017	1.00	25.63
ATOM	570	CD1	PHE	232	58.000	32.967	12.785	1.00	24.50
ATOM	571	CD2	PHE	232	57.980	32.830	15.181	1.00	19.35
ATOM	572	CE1	PHE	232	58.381	31.630	12.705	1.00	22.27
ATOM	573	CE2	PHE	232	58.359	31.496	15.114	1.00	20.63
ATOM	574	CZ	PHE	232	58.561	30.893	13.873	1.00	26.10
ATOM	575	C	PHE	232	55.018	34.093	14.328	1.00	23.51
ATOM	576	O	PHE	232	54.541	33.189	13.637	1.00	22.39
ATOM	577	N	ALA	233	54.837	34.182	15.644	1.00	24.55
ATOM	578	CA	ALA	233	54.070	33.192	16.387	1.00	23.10
ATOM	579	CB	ALA	233	54.145	33.490	17.869	1.00	17.99
ATOM	580	C	ALA	233	52.616	33.137	15.929	1.00	27.99
ATOM	581	O	ALA	233	52.063	32.051	15.744	1.00	25.71
ATOM	582	N	LYS	234	51.997	34.305	15.760	1.00	30.19
ATOM	583	CA	LYS	234	50.601	34.380	15.325	1.00	31.58
ATOM	584	CB	LYS	234	50.136	35.838	15.229	1.00	30.40
ATOM	585	CG	LYS	234	50.100	36.593	16.555	1.00	37.97
ATOM	586	CD	LYS	234	49.151	35.947	17.569	1.00	53.64
ATOM	587	CE	LYS	234	47.694	35.958	17.101	1.00	59.60
ATOM	588	NZ	LYS	234	46.773	35.268	18.060	1.00	54.22
ATOM	589	C	LYS	234	50.388	33.686	13.978	1.00	30.35
ATOM	590	O	LYS	234	49.318	33.142	13.716	1.00	32.50
ATOM	591	N	LYS	235	51.425	33.687	13.144	1.00	23.98
ATOM	592	CA	LYS	235	51.351	33.071	11.828	1.00	22.75
ATOM	593	CB	LYS	235	52.353	33.737	10.896	1.00	23.12
ATOM	594	CG	LYS	235	51.997	35.181	10.631	1.00	20.88
ATOM	595	CD	LYS	235	52.982	35.836	9.688	1.00	26.50
ATOM	596	CE	LYS	235	52.512	37.227	9.310	1.00	31.33
ATOM	597	NZ	LYS	235	53.439	37.862	8.341	1.00	36.51
ATOM	598	C	LYS	235	51.508	31.554	11.791	1.00	28.37
ATOM	599	O	LYS	235	51.491	30.948	10.721	1.00	29.62
ATOM	600	N	LEU	236	51.700	30.943	12.954	1.00	33.22
ATOM	601	CA	LEU	236	51.828	29.494	13.036	1.00	32.24
ATOM	602	CB	LEU	236	52.911	29.101	14.043	1.00	26.25
ATOM	603	CG	LEU	236	54.327	29.582	13.730	1.00	23.40
ATOM	604	CD1	LEU	236	55.289	29.113	14.806	1.00	20.52
ATOM	605	CD2	LEU	236	54.750	29.054	12.374	1.00	20.29
ATOM	606	C	LEU	236	50.470	28.984	13.502	1.00	37.08
ATOM	607	O	LEU	236	50.013	29.342	14.588	1.00	34.23
ATOM	608	N	PRO	237	49.811	28.134	12.695	1.00	44.89
ATOM	609	CD	PRO	237	50.351	27.597	11.432	1.00	42.95
ATOM	610	CA	PRO	237	48.491	27.556	12.990	1.00	48.88
ATOM	611	CB	PRO	237	48.396	26.406	11.987	1.00	51.40
ATOM	612	CG	PRO	237	49.142	26.931	10.813	1.00	53.54
ATOM	613	C	PRO	237	48.278	27.072	14.430	1.00	49.12
ATOM	614	O	PRO	237	47.387	27.551	15.133	1.00	48.18

ATOM	615	N	MET	238	49.104	26.126	14.860	1.00	45.79
ATOM	616	CA	MET	238	49.029	25.558	16.200	1.00	52.79
ATOM	617	CB	MET	238	50.133	24.505	16.378	1.00	49.72
ATOM	618	CG	MET	238	49.861	23.195	15.637	1.00	58.16
ATOM	619	SD	MET	238	51.342	22.205	15.284	1.00	60.11
ATOM	620	CE	MET	238	50.993	21.626	13.625	1.00	53.03
ATOM	621	C	MET	238	49.103	26.593	17.324	1.00	53.36
ATOM	622	O	MET	238	48.583	26.365	18.420	1.00	58.87
ATOM	623	N	PHE	239	49.713	27.742	17.043	1.00	48.09
ATOM	624	CA	PHE	239	49.861	28.793	18.045	1.00	41.38
ATOM	625	CB	PHE	239	51.011	29.736	17.677	1.00	32.92
ATOM	626	CG	PHE	239	51.307	30.763	18.734	1.00	31.32
ATOM	627	CD1	PHE	239	52.162	30.462	19.790	1.00	28.28
ATOM	628	CD2	PHE	239	50.715	32.024	18.689	1.00	24.80
ATOM	629	CE1	PHE	239	52.425	31.402	20.790	1.00	29.45
ATOM	630	CE2	PHE	239	50.970	32.973	19.682	1.00	32.29
ATOM	631	CZ	PHE	239	51.828	32.659	20.737	1.00	26.00
ATOM	632	C	PHE	239	48.590	29.592	18.344	1.00	37.40
ATOM	633	O	PHE	239	48.194	29.696	19.501	1.00	33.32
ATOM	634	N	SER	240	47.958	30.166	17.321	1.00	36.32
ATOM	635	CA	SER	240	46.745	30.959	17.529	1.00	39.00
ATOM	636	CB	SER	240	46.385	31.724	16.258	1.00	47.52
ATOM	637	OG	SER	240	47.390	32.671	15.947	1.00	52.67
ATOM	638	C	SER	240	45.539	30.158	18.032	1.00	36.82
ATOM	639	O	SER	240	44.548	30.743	18.485	1.00	43.02
ATOM	640	N	GLU	241	45.617	28.833	17.931	1.00	38.98
ATOM	641	CA	GLU	241	44.554	27.954	18.408	1.00	40.35
ATOM	642	CB	GLU	241	44.788	26.521	17.926	1.00	49.38
ATOM	643	CG	GLU	241	44.541	26.287	16.452	1.00	65.25
ATOM	644	CD	GLU	241	44.873	24.856	16.002	1.00	70.72
ATOM	645	OE1	GLU	241	44.806	23.923	16.845	1.00	73.36
ATOM	646	OE2	GLU	241	45.211	24.679	14.805	1.00	68.60
ATOM	647	C	GLU	241	44.550	27.968	19.934	1.00	37.83
ATOM	648	O	GLU	241	43.504	27.857	20.570	1.00	40.77
ATOM	649	N	LEU	242	45.747	28.103	20.498	1.00	34.71
ATOM	650	CA	LEU	242	45.974	28.132	21.944	1.00	31.77
ATOM	651	CB	LEU	242	47.478	28.240	22.215	1.00	24.87
ATOM	652	CG	LEU	242	48.345	27.006	22.455	1.00	30.51
ATOM	653	CD1	LEU	242	47.814	25.763	21.772	1.00	31.72
ATOM	654	CD2	LEU	242	49.743	27.328	21.996	1.00	24.25
ATOM	655	C	LEU	242	45.274	29.287	22.657	1.00	29.41
ATOM	656	O	LEU	242	45.029	30.339	22.071	1.00	28.12
ATOM	657	N	PRO	243	44.913	29.089	23.938	1.00	32.37
ATOM	658	CD	PRO	243	44.976	27.849	24.728	1.00	27.94
ATOM	659	CA	PRO	243	44.253	30.165	24.685	1.00	33.92
ATOM	660	CB	PRO	243					



ATOM	662	C	PRO	243	45.246	31.334	24.775	1.00	35.86
ATOM	663	O	PRO	243	46.461	31.110	24.809	1.00	38.79
ATOM	664	N	CYS	244	44.751	32.570	24.834	1.00	39.67
ATOM	665	CA	CYS	244	45.621	33.749	24.931	1.00	45.78
ATOM	666	CB	CYS	244	44.788	35.028	25.102	1.00	71.13
ATOM	667	SG	CYS	244	44.068	35.680	23.580	1.00	100.76
ATOM	669	C	CYS	244	46.660	33.665	26.051	1.00	40.08
ATOM	670	O	CYS	244	47.797	34.096	25.879	1.00	35.68
ATOM	671	N	GLU	245	46.265	33.088	27.184	1.00	34.25
ATOM	672	CA	GLU	245	47.156	32.939	28.337	1.00	34.60
ATOM	673	CB	GLU	245	46.426	32.296	29.524	1.00	42.20
ATOM	674	CG	GLU	245	45.356	33.171	30.160	1.00	41.92
ATOM	675	CD	GLU	245	43.947	32.808	29.730	1.00	39.68
ATOM	676	OE1	GLU	245	43.080	32.693	30.618	1.00	38.31
ATOM	677	OE2	GLU	245	43.697	32.644	28.516	1.00	48.13
ATOM	678	C	GLU	245	48.376	32.109	27.984	1.00	29.54
ATOM	679	O	GLU	245	49.497	32.437	28.381	1.00	33.54
ATOM	680	N	ASP	246	48.146	31.034	27.236	1.00	26.40
ATOM	681	CA	ASP	246	49.219	30.154	26.794	1.00	26.99
ATOM	682	CB	ASP	246	48.650	28.887	26.153	1.00	29.86
ATOM	683	CG	ASP	246	48.184	27.876	27.175	1.00	34.10
ATOM	684	OD1	ASP	246	48.149	28.199	28.381	1.00	31.83
ATOM	685	OD2	ASP	246	47.863	26.742	26.772	1.00	35.79
ATOM	686	C	ASP	246	50.103	30.875	25.790	1.00	28.07
ATOM	687	O	ASP	246	51.331	30.789	25.863	1.00	27.35
ATOM	688	N	GLN	247	49.472	31.577	24.851	1.00	25.53
ATOM	689	CA	GLN	247	50.198	32.327	23.829	1.00	26.08
ATOM	690	CB	GLN	247	49.228	33.089	22.924	1.00	23.38
ATOM	691	CG	GLN	247	48.303	32.213	22.091	1.00	23.76
ATOM	692	CD	GLN	247	47.429	33.029	21.151	1.00	26.89
ATOM	693	OE1	GLN	247	47.853	34.054	20.628	1.00	33.51
ATOM	694	NE2	GLN	247	46.198	32.593	20.957	1.00	27.44
ATOM	695	C	GLN	247	51.133	33.313	24.511	1.00	22.74
ATOM	696	O	GLN	247	52.326	33.373	24.205	1.00	27.63
ATOM	697	N	ILE	248	50.588	34.047	25.473	1.00	25.03
ATOM	698	CA	ILE	248	51.353	35.035	26.220	1.00	25.94
ATOM	699	CB	ILE	248	50.436	35.781	27.226	1.00	24.84
ATOM	700	CG2	ILE	248	51.251	36.633	28.179	1.00	21.87
ATOM	701	CG1	ILE	248	49.430	36.652	26.459	1.00	27.98
ATOM	702	CD1	ILE	248	48.359	37.298	27.328	1.00	29.90
ATOM	703	C	ILE	248	52.535	34.382	26.939	1.00	27.53
ATOM	704	O	ILE	248	53.671	34.847	26.833	1.00	29.35
ATOM	705	N	ILE	249	52.279	33.274	27.622	1.00	24.38
ATOM	706	CA	ILE	249	53.334	32.582	28.354	1.00	26.26
ATOM	707	CB	ILE	249	52.759	31.395	29.166	1.00	29.81
ATOM	708	CG2	ILE	249					



ATOM	710	CD1 ILE	249	51.173	30.838	31.076	1.00	32.35
ATOM	711	C ILE	249	54.448	32.103	27.422	1.00	27.78
ATOM	712	O ILE	249	55.634	32.297	27.708	1.00	29.37
ATOM	713	N LEU	250	54.061	31.516	26.289	1.00	29.25
ATOM	714	CA LEU	250	55.021	31.005	25.319	1.00	24.49
ATOM	715	CB LEU	250	54.303	30.224	24.214	1.00	23.75
ATOM	716	CG LEU	250	53.541	28.962	24.629	1.00	23.18
ATOM	717	CD1 LEU	250	52.886	28.353	23.416	1.00	19.94
ATOM	718	CD2 LEU	250	54.475	27.960	25.278	1.00	20.76
ATOM	719	C LEU	250	55.878	32.116	24.714	1.00	22.20
ATOM	720	O LEU	250	57.082	31.940	24.528	1.00	23.49
ATOM	721	N LEU	251	55.256	33.249	24.399	1.00	24.21
ATOM	722	CA LEU	251	55.980	34.384	23.831	1.00	27.98
ATOM	723	CB LEU	251	55.010	35.488	23.408	1.00	25.91
ATOM	724	CG LEU	251	54.287	35.245	22.085	1.00	29.46
ATOM	725	CD1 LEU	251	53.121	36.217	21.939	1.00	35.03
ATOM	726	CD2 LEU	251	55.268	35.364	20.924	1.00	23.65
ATOM	727	C LEU	251	56.998	34.931	24.828	1.00	26.85
ATOM	728	O LEU	251	58.165	35.143	24.484	1.00	23.12
ATOM	729	N LYS	252	56.556	35.145	26.063	1.00	25.33
ATOM	730	CA LYS	252	57.427	35.644	27.119	1.00	31.33
ATOM	731	CB LYS	252	56.659	35.723	28.437	1.00	37.06
ATOM	732	CG LYS	252	55.593	36.805	28.511	1.00	41.75
ATOM	733	CD LYS	252	54.779	36.619	29.783	1.00	52.64
ATOM	734	CE LYS	252	53.822	37.767	30.057	1.00	62.60
ATOM	735	NZ LYS	252	54.503	39.005	30.520	1.00	71.68
ATOM	736	C LYS	252	58.622	34.705	27.293	1.00	29.08
ATOM	737	O LYS	252	59.758	35.150	27.460	1.00	35.24
ATOM	738	N GLY	253	58.355	33.403	27.211	1.00	24.98
ATOM	739	CA GLY	253	59.407	32.416	27.369	1.00	22.80
ATOM	740	C GLY	253	60.413	32.282	26.235	1.00	26.90
ATOM	741	O GLY	253	61.572	31.948	26.489	1.00	31.90
ATOM	742	N CYS	254	60.013	32.574	24.997	1.00	25.42
ATOM	743	CA CYS	254	60.932	32.427	23.863	1.00	20.71
ATOM	744	CB CYS	254	60.314	31.509	22.811	1.00	24.98
ATOM	745	SG CYS	254	58.976	32.310	21.909	1.00	24.24
ATOM	746	C CYS	254	61.353	33.716	23.164	1.00	22.79
ATOM	747	O CYS	254	62.217	33.683	22.282	1.00	23.23
ATOM	748	N CYS	255	60.757	34.842	23.539	1.00	21.47
ATOM	749	CA CYS	255	61.061	36.114	22.884	1.00	22.50
ATOM	750	CB CYS	255	60.318	37.262	23.567	1.00	21.72
ATOM	751	SG CYS	255	60.353	38.768	22.597	1.00	24.73
ATOM	752	C CYS	255	62.547	36.457	22.738	1.00	23.81
ATOM	753	O CYS	255	63.015	36.746	21.632	1.00	23.48
ATOM	754	N MET	256	63.294	36.402	23.838	1.00	22.13
ATOM	755	CA MET	256	64.719	36.713	23.792	1.00	22.91
ATOM	756	CB MET	256	65.286	36.810	25.213	1.00	23.78

ATOM	757	CG	MET	256	66.781	37.094	25.272	1.00	17.41
ATOM	758	SD	MET	256	67.196	38.632	24.415	1.00	23.65
ATOM	759	CE	MET	256	69.010	38.715	24.624	1.00	18.57
ATOM	760	C	MET	256	65.487	35.671	22.980	1.00	21.41
ATOM	761	O	MET	256	66.432	36.005	22.260	1.00	22.01
ATOM	762	N-	GLU	257	65.058	34.415	23.068	1.00	23.18
ATOM	763	CA	GLU	257	65.705	33.323	22.345	1.00	22.90
ATOM	764	CB	GLU	257	65.085	31.989	22.753	1.00	24.00
ATOM	765	CG	GLU	257	65.522	31.521	24.125	1.00	33.44
ATOM	766	CD	GLU	257	64.564	30.527	24.735	1.00	38.03
ATOM	767	OE1	GLU	257	63.977	29.705	24.000	1.00	45.59
ATOM	768	OE2	GLU	257	64.385	30.577	25.965	1.00	45.75
ATOM	769	C	GLU	257	65.595	33.526	20.840	1.00	21.68
ATOM	770	O	GLU	257	66.586	33.421	20.107	1.00	20.02
ATOM	771	N	ILE	258	64.383	33.852	20.391	1.00	17.07
ATOM	772	CA	ILE	258	64.135	34.090	18.973	1.00	17.01
ATOM	773	CB	ILE	258	62.613	34.207	18.684	1.00	17.33
ATOM	774	CG2	ILE	258	62.369	34.758	17.276	1.00	15.91
ATOM	775	CG1	ILE	258	61.952	32.831	18.885	1.00	16.69
ATOM	776	CD1	ILE	258	60.450	32.783	18.632	1.00	16.31
ATOM	777	C	ILE	258	64.911	35.324	18.501	1.00	17.65
ATOM	778	O	ILE	258	65.605	35.263	17.484	1.00	22.58
ATOM	779	N	MET	259	64.865	36.410	19.274	1.00	20.17
ATOM	780	CA	MET	259	65.584	37.628	18.909	1.00	15.03
ATOM	781	CB	MET	259	65.234	38.771	19.856	1.00	20.12
ATOM	782	CG	MET	259	63.791	39.191	19.775	1.00	17.19
ATOM	783	SD	MET	259	63.523	40.795	20.524	1.00	28.92
ATOM	784	CE	MET	259	63.718	40.406	22.261	1.00	19.58
ATOM	785	C	MET	259	67.090	37.402	18.884	1.00	18.84
ATOM	786	O	MET	259	67.783	37.912	17.996	1.00	29.07
ATOM	787	N	SER	260	67.590	36.618	19.837	1.00	21.45
ATOM	788	CA	SER	260	69.019	36.319	19.906	1.00	18.71
ATOM	789	CB	SER	260	69.367	35.595	21.207	1.00	18.35
ATOM	790	OG	SER	260	69.128	36.421	22.329	1.00	25.42
ATOM	791	C	SER	260	69.430	35.469	18.709	1.00	17.83
ATOM	792	O	SER	260	70.497	35.673	18.131	1.00	22.97
ATOM	793	N	LEU	261	68.572	34.522	18.331	1.00	21.66
ATOM	794	CA	LEU	261	68.837	33.663	17.179	1.00	20.98
ATOM	795	CB	LEU	261	67.739	32.608	17.053	1.00	22.66
ATOM	796	CG	LEU	261	67.719	31.759	15.781	1.00	22.12
ATOM	797	CD1	LEU	261	68.998	30.938	15.665	1.00	18.51
ATOM	798	CD2	LEU	261	66.498	30.851	15.800	1.00	19.60
ATOM	799	C	LEU	261	68.873	34.527	15.920	1.00	22.95
ATOM	800	O	LEU	261	69.779	34.402	15.091	1.00	22.62
ATOM	801	N	ARG	262	67.892	35.418	15.798	1.00	22.12
ATOM	802	CA	ARG	262					

ATOM	804	CG	ARG	262	65.304	36.268	14.362	1.00	21.48
ATOM	805	CD	ARG	262	64.026	37.077	14.345	1.00	19.12
ATOM	806	NE	ARG	262	62.990	36.377	13.599	1.00	22.18
ATOM	807	CZ	ARG	262	61.780	36.862	13.333	1.00	22.88
ATOM	808	NH1	ARG	262	61.429	38.075	13.752	1.00	20.81
ATOM	809	NH2	ARG	262	60.912	36.129	12.648	1.00	20.26
ATOM	810	C	ARG	262	69.044	37.196	14.531	1.00	25.05
ATOM	811	O	ARG	262	69.485	37.513	13.427	1.00	22.98
ATOM	812	N	ALA	263	69.608	37.579	15.676	1.00	26.36
ATOM	813	CA	ALA	263	70.818	38.400	15.705	1.00	27.02
ATOM	814	CB	ALA	263	70.997	39.045	17.087	1.00	25.80
ATOM	815	C	ALA	263	72.026	37.514	15.368	1.00	25.21
ATOM	816	O	ALA	263	72.825	37.844	14.492	1.00	31.14
ATOM	817	N	ALA	264	72.109	36.358	16.027	1.00	25.62
ATOM	818	CA	ALA	264	73.203	35.408	15.828	1.00	23.85
ATOM	819	CB	ALA	264	73.062	34.237	16.794	1.00	17.15
ATOM	820	C	ALA	264	73.345	34.901	14.391	1.00	26.03
ATOM	821	O	ALA	264	74.460	34.773	13.886	1.00	25.66
ATOM	822	N	VAL	265	72.234	34.615	13.723	1.00	25.22
ATOM	823	CA	VAL	265	72.327	34.128	12.350	1.00	28.38
ATOM	824	CB	VAL	265	71.028	33.457	11.857	1.00	24.59
ATOM	825	CG1	VAL	265	70.707	32.264	12.719	1.00	25.53
ATOM	826	CG2	VAL	265	69.881	34.440	11.853	1.00	20.86
ATOM	827	C	VAL	265	72.747	35.235	11.393	1.00	31.46
ATOM	828	O	VAL	265	73.024	34.973	10.222	1.00	34.75
ATOM	829	N	ARG	266	72.795	36.464	11.896	1.00	30.10
ATOM	830	CA	ARG	266	73.211	37.602	11.089	1.00	30.69
ATOM	831	CB	ARG	266	72.170	38.713	11.148	1.00	25.13
ATOM	832	CG	ARG	266	70.976	38.406	10.299	1.00	25.43
ATOM	833	CD	ARG	266	69.999	39.537	10.277	1.00	29.56
ATOM	834	NE	ARG	266	69.032	39.340	9.205	1.00	31.59
ATOM	835	CZ	ARG	266	67.814	39.861	9.197	1.00	31.18
ATOM	836	NH1	ARG	266	67.408	40.611	10.215	1.00	31.01
ATOM	837	NH2	ARG	266	67.012	39.648	8.163	1.00	28.21
ATOM	838	C	ARG	266	74.568	38.111	11.544	1.00	34.28
ATOM	839	O	ARG	266	74.877	39.300	11.423	1.00	41.19
ATOM	840	N	TYR	267	75.362	37.207	12.108	1.00	30.80
ATOM	841	CA	TYR	267	76.694	37.544	12.573	1.00	33.84
ATOM	842	CB	TYR	267	77.202	36.461	13.534	1.00	32.56
ATOM	843	CG	TYR	267	78.674	36.570	13.867	1.00	34.23
ATOM	844	CD1	TYR	267	79.131	37.465	14.835	1.00	32.60
ATOM	845	CE1	TYR	267	80.491	37.593	15.106	1.00	34.90
ATOM	846	CD2	TYR	267	79.615	35.801	13.184	1.00	32.84
ATOM	847	CE2	TYR	267	80.972	35.920	13.446	1.00	34.70
ATOM	848	CZ	TYR	267	81.404	36.816	14.405	1.00	36.21
ATOM	849	OH	TYR	267	82.749	36.940	14.651	1.00	39.48
ATOM	850	C	TYR	267	77.615	37.649	11.360	1.00	37.82

ATOM	851	O	TYR	267	77.648	36.749	10.517	1.00	39.45
ATOM	852	N	ASP	268	78.319	38.769	11.239	1.00	44.62
ATOM	853	CA	ASP	268	79.248	38.963	10.133	1.00	45.56
ATOM	854	CB	ASP	268	79.096	40.366	9.533	1.00	46.62
ATOM	855	CG	ASP	268	80.068	40.624	8.391	1.00	50.96
ATOM	856	OD1	ASP	268	80.204	39.755	7.502	1.00	55.65
ATOM	857	OD2	ASP	268	80.700	41.699	8.384	1.00	52.09
ATOM	858	C	ASP	268	80.675	38.751	10.630	1.00	44.44
ATOM	859	O	ASP	268	81.242	39.614	11.304	1.00	45.68
ATOM	860	N	PRO	269	81.281	37.600	10.296	1.00	45.94
ATOM	861	CD	PRO	269	80.739	36.503	9.476	1.00	43.72
ATOM	862	CA	PRO	269	82.651	37.309	10.730	1.00	46.63
ATOM	863	CB	PRO	269	82.884	35.889	10.208	1.00	43.88
ATOM	864	CG	PRO	269	81.983	35.797	9.018	1.00	44.66
ATOM	865	C	PRO	269	83.682	38.298	10.190	1.00	50.80
ATOM	866	O	PRO	269	84.681	38.578	10.854	1.00	48.56
ATOM	867	N	ALA	270	83.407	38.858	9.012	1.00	55.09
ATOM	868	CA	ALA	270	84.306	39.820	8.374	1.00	55.68
ATOM	869	CB	ALA	270	83.799	40.168	6.974	1.00	53.64
ATOM	870	C	ALA	270	84.528	41.096	9.196	1.00	56.18
ATOM	871	O	ALA	270	85.577	41.729	9.082	1.00	61.07
ATOM	872	N	SER	271	83.543	41.479	10.006	1.00	51.38
ATOM	873	CA	SER	271	83.661	42.678	10.836	1.00	45.90
ATOM	874	CB	SER	271	82.710	43.774	10.346	1.00	44.49
ATOM	875	OG	SER	271	81.360	43.358	10.404	1.00	45.26
ATOM	876	C	SER	271	83.409	42.395	12.317	1.00	46.61
ATOM	877	O	SER	271	83.431	43.309	13.143	1.00	48.31
ATOM	878	N	ASP	272	83.172	41.126	12.642	1.00	46.73
ATOM	879	CA	ASP	272	82.920	40.689	14.013	1.00	42.49
ATOM	880	CB	ASP	272	84.200	40.807	14.849	1.00	42.12
ATOM	881	CG	ASP	272	84.103	40.072	16.169	1.00	50.30
ATOM	882	OD1	ASP	272	83.417	39.028	16.218	1.00	45.10
ATOM	883	OD2	ASP	272	84.708	40.537	17.160	1.00	57.61
ATOM	884	C	ASP	272	81.769	41.465	14.658	1.00	40.95
ATOM	885	O	ASP	272	81.885	41.975	15.779	1.00	42.93
ATOM	886	N	THR	273	80.651	41.531	13.945	1.00	38.57
ATOM	887	CA	THR	273	79.473	42.239	14.425	1.00	40.99
ATOM	888	CB	THR	273	79.262	43.574	13.656	1.00	40.76
ATOM	889	OG1	THR	273	79.240	43.318	12.248	1.00	42.61
ATOM	890	CG2	THR	273	80.373	44.574	13.965	1.00	39.67
ATOM	891	C	THR	273	78.210	41.397	14.251	1.00	39.94
ATOM	892	O	THR	273	78.202	40.419	13.494	1.00	36.66
ATOM	893	N	LEU	274	77.168	41.757	14.993	1.00	36.08
ATOM	894	CA	LEU	274	75.867	41.096	14.907	1.00	34.28
ATOM	895	CB	LEU	274	75.343	40.699	16.292	1.00	30.96
ATOM	896	CG	LEU	274	75.952	39.536	17.0		



ATOM	898	CD2 LEU	274	75.744	38.237	16.309	1.00	27.43
ATOM	899	C LEU	274	74.943	42.163	14.347	1.00	36.49
ATOM	900	O LEU	274	75.152	43.354	14.596	1.00	40.27
ATOM	901	N THR	275	73.923	41.758	13.606	1.00	36.42
ATOM	902	CA THR	275	72.994	42.731	13.062	1.00	35.07
ATOM	903	CB THR	275	72.773	42.522	11.556	1.00	36.04
ATOM	904	OG1 THR	275	74.028	42.625	10.875	1.00	41.52
ATOM	905	CG2 THR	275	71.852	43.583	11.008	1.00	36.47
ATOM	906	C THR	275	71.673	42.655	13.814	1.00	34.32
ATOM	907	O THR	275	71.055	41.590	13.907	1.00	34.96
ATOM	908	N LEU	276	71.292	43.767	14.432	1.00	31.79
ATOM	909	CA LEU	276	70.044	43.840	15.173	1.00	29.47
ATOM	910	CB LEU	276	70.181	44.766	16.389	1.00	25.29
ATOM	911	CG LEU	276	71.328	44.501	17.383	1.00	29.01
ATOM	912	CD1 LEU	276	71.179	45.410	18.594	1.00	20.92
ATOM	913	CD2 LEU	276	71.358	43.042	17.834	1.00	22.79
ATOM	914	C LEU	276	68.966	44.350	14.228	1.00	31.69
ATOM	915	O LEU	276	69.175	45.335	13.510	1.00	33.87
ATOM	916	N SER	277	67.862	43.608	14.162	1.00	33.07
ATOM	917	CA SER	277	66.721	43.935	13.315	1.00	30.61
ATOM	918	CB SER	277	65.949	45.111	13.909	1.00	22.87
ATOM	919	OG SER	277	65.587	44.822	15.250	1.00	23.35
ATOM	920	C SER	277	67.103	44.200	11.860	1.00	31.85
ATOM	921	O SER	277	66.433	44.958	11.158	1.00	32.13
ATOM	922	N GLY	278	68.188	43.566	11.421	1.00	32.29
ATOM	923	CA GLY	278	68.664	43.716	10.058	1.00	37.59
ATOM	924	C GLY	278	69.063	45.122	9.639	1.00	43.26
ATOM	925	O GLY	278	69.313	45.358	8.455	1.00	42.60
ATOM	926	N GLU	279	69.177	46.038	10.599	1.00	43.42
ATOM	927	CA GLU	279	69.532	47.420	10.291	1.00	44.55
ATOM	928	CB GLU	279	68.292	48.310	10.394	1.00	44.66
ATOM	929	CG GLU	279	67.671	48.344	11.783	1.00	54.19
ATOM	930	CD GLU	279	66.400	49.171	11.845	1.00	64.96
ATOM	931	OE1 GLU	279	65.627	49.174	10.859	1.00	71.43
ATOM	932	OE2 GLU	279	66.167	49.814	12.891	1.00	66.65
ATOM	933	C GLU	279	70.654	48.019	11.133	1.00	45.52
ATOM	934	O GLU	279	71.207	49.057	10.772	1.00	51.83
ATOM	935	N MET	280	71.007	47.373	12.242	1.00	44.66
ATOM	936	CA MET	280	72.060	47.904	13.105	1.00	34.22
ATOM	937	CB MET	280	71.470	48.382	14.433	1.00	32.38
ATOM	938	CG MET	280	72.479	49.058	15.345	1.00	37.87
ATOM	939	SD MET	280	71.912	49.201	17.052	1.00	41.78
ATOM	940	CE MET	280	70.650	50.495	16.911	1.00	37.01
ATOM	941	C MET	280	73.183	46.920	13.386	1.00	35.70
ATOM	942	O MET	280	72.976	45.900	14.044	1.00	36.99
ATOM	943	N ALA	281	74.366	47.221	12.867	1.00	34.80
ATOM	944	CA ALA	281	75.535	46.377	13.091	1.00	35.11



ATOM	945	CB	ALA	281	76.529	46.527	11.955	1.00	31.27
ATOM	946	C	ALA	281	76.155	46.837	14.406	1.00	35.96
ATOM	947	O	ALA	281	76.478	48.015	14.570	1.00	39.10
ATOM	948	N	VAL	282	76.285	45.916	15.353	1.00	36.46
ATOM	949	CA	VAL	282	76.839	46.246	16.655	1.00	36.05
ATOM	950	CB	VAL	282	75.783	46.090	17.783	1.00	35.60
ATOM	951	CG1	VAL	282	74.633	47.069	17.568	1.00	38.73
ATOM	952	CG2	VAL	282	75.262	44.660	17.844	1.00	33.27
ATOM	953	C	VAL	282	78.062	45.408	16.996	1.00	37.70
ATOM	954	O	VAL	282	78.137	44.223	16.660	1.00	37.45
ATOM	955	N	ALA	283	79.032	46.047	17.637	1.00	39.21
ATOM	956	CA	ALA	283	80.254	45.375	18.048	1.00	43.73
ATOM	957	CB	ALA	283	81.433	46.352	18.047	1.00	42.04
ATOM	958	C	ALA	283	80.060	44.752	19.435	1.00	43.28
ATOM	959	O	ALA	283	79.179	45.157	20.203	1.00	45.77
ATOM	960	N	ARG	284	80.903	43.774	19.744	1.00	41.96
ATOM	961	CA	ARG	284	80.866	43.044	21.004	1.00	44.87
ATOM	962	CB	ARG	284	82.084	42.125	21.087	1.00	46.34
ATOM	963	CG	ARG	284	81.930	40.947	22.017	1.00	51.85
ATOM	964	CD	ARG	284	83.107	40.010	21.844	1.00	60.73
ATOM	965	NE	ARG	284	83.262	39.571	20.455	1.00	54.30
ATOM	966	CZ	ARG	284	83.221	38.300	20.074	1.00	53.66
ATOM	967	NH1	ARG	284	83.032	37.343	20.973	1.00	49.99
ATOM	968	NH2	ARG	284	83.379	37.984	18.797	1.00	47.31
ATOM	969	C	ARG	284	80.803	43.945	22.237	1.00	44.85
ATOM	970	O	ARG	284	79.896	43.806	23.062	1.00	48.26
ATOM	971	N	GLU	285	81.750	44.873	22.349	1.00	41.60
ATOM	972	CA	GLU	285	81.802	45.787	23.484	1.00	41.17
ATOM	973	CB	GLU	285	83.043	46.675	23.392	1.00	39.97
ATOM	974	C	GLU	285	80.538	46.640	23.603	1.00	40.08
ATOM	975	O	GLU	285	80.023	46.849	24.703	1.00	41.16
ATOM	976	N	GLN	286	80.017	47.088	22.463	1.00	38.49
ATOM	977	CA	GLN	286	78.818	47.926	22.425	1.00	36.25
ATOM	978	CB	GLN	286	78.549	48.401	20.997	1.00	39.50
ATOM	979	CG	GLN	286	79.619	49.311	20.424	1.00	43.62
ATOM	980	CD	GLN	286	79.324	49.710	18.987	1.00	49.48
ATOM	981	OE1	GLN	286	79.253	48.856	18.097	1.00	48.41
ATOM	982	NE2	GLN	286	79.125	51.000	18.755	1.00	47.15
ATOM	983	C	GLN	286	77.563	47.255	22.988	1.00	35.40
ATOM	984	O	GLN	286	76.903	47.806	23.871	1.00	31.24
ATOM	985	N	LEU	287	77.234	46.071	22.480	1.00	32.96
ATOM	986	CA	LEU	287	76.055	45.349	22.950	1.00	33.40
ATOM	987	CB	LEU	287	75.767	44.138	22.054	1.00	28.67
ATOM	988	CG	LEU	287	74.466	43.375	22.342	1.00	26.66
ATOM	989	CD1	LEU	287	73.263	44.305	22.244	1.00	19.41
ATOM	990	CD2	LEU	287</					

ATOM	992	O	LEU	287	75.265	44.857	25.175	1.00	33.92
ATOM	993	N	LYS	288	77.476	44.621	24.781	1.00	35.38
ATOM	994	CA	LYS	288	77.814	44.204	26.140	1.00	36.12
ATOM	995	CB	LYS	288	79.296	43.839	26.210	1.00	37.13
ATOM	996	CG	LYS	288	79.762	43.280	27.533	1.00	44.61
ATOM	997	CD	LYS	288	81.256	43.018	27.494	1.00	54.07
ATOM	998	CE	LYS	288	81.757	42.435	28.801	1.00	60.87
ATOM	999	NZ	LYS	288	81.291	41.041	29.039	1.00	61.53
ATOM	1000	C	LYS	288	77.510	45.345	27.109	1.00	36.90
ATOM	1001	O	LYS	288	76.684	45.206	28.013	1.00	40.68
ATOM	1002	N	ASN	289	78.129	46.495	26.863	1.00	35.94
ATOM	1003	CA	ASN	289	77.947	47.680	27.695	1.00	36.12
ATOM	1004	CB	ASN	289	78.982	48.738	27.332	1.00	31.78
ATOM	1005	CG	ASN	289	80.388	48.263	27.569	1.00	40.31
ATOM	1006	OD1	ASN	289	80.627	47.422	28.440	1.00	43.12
ATOM	1007	ND2	ASN	289	81.326	48.758	26.775	1.00	35.36
ATOM	1008	C	ASN	289	76.553	48.277	27.590	1.00	36.98
ATOM	1009	O	ASN	289	76.099	48.959	28.509	1.00	34.29
ATOM	1010	N	GLY	290	75.883	48.032	26.466	1.00	32.65
ATOM	1011	CA	GLY	290	74.541	48.550	26.256	1.00	28.61
ATOM	1012	C	GLY	290	73.497	48.001	27.210	1.00	26.54
ATOM	1013	O	GLY	290	72.362	48.480	27.234	1.00	31.06
ATOM	1014	N	GLY	291	73.861	46.978	27.977	1.00	28.89
ATOM	1015	CA	GLY	291	72.929	46.413	28.937	1.00	25.24
ATOM	1016	C	GLY	291	72.872	44.900	28.997	1.00	28.12
ATOM	1017	O	GLY	291	72.335	44.345	29.955	1.00	31.16
ATOM	1018	N	LEU	292	73.406	44.223	27.985	1.00	29.51
ATOM	1019	CA	LEU	292	73.361	42.766	27.969	1.00	32.79
ATOM	1020	CB	LEU	292	73.304	42.240	26.531	1.00	28.00
ATOM	1021	CG	LEU	292	71.948	42.355	25.827	1.00	23.68
ATOM	1022	CD1	LEU	292	72.004	41.626	24.509	1.00	26.12
ATOM	1023	CD2	LEU	292	70.851	41.764	26.694	1.00	23.36
ATOM	1024	C	LEU	292	74.484	42.085	28.742	1.00	32.33
ATOM	1025	O	LEU	292	74.312	40.967	29.232	1.00	32.22
ATOM	1026	N	GLY	293	75.627	42.750	28.846	1.00	30.31
ATOM	1027	CA	GLY	293	76.751	42.176	29.561	1.00	28.82
ATOM	1028	C	GLY	293	77.238	40.894	28.913	1.00	29.87
ATOM	1029	O	GLY	293	77.432	40.843	27.698	1.00	35.43
ATOM	1030	N	VAL	294	77.392	39.848	29.714	1.00	31.88
ATOM	1031	CA	VAL	294	77.866	38.561	29.217	1.00	35.77
ATOM	1032	CB	VAL	294	78.232	37.590	30.363	1.00	34.29
ATOM	1033	CG1	VAL	294	79.462	38.092	31.095	1.00	37.54
ATOM	1034	CG2	VAL	294	77.065	37.425	31.322	1.00	25.62
ATOM	1035	C	VAL	294	76.882	37.879	28.274	1.00	35.89
ATOM	1036	O	VAL	294	77.263	36.960	27.541	1.00	37.

ATOM	1039	CB	VAL	295	73.208	38.298	27.677	1.00	31.25
ATOM	1040	CG1	VAL	295	72.208	37.706	26.694	1.00	23.54
ATOM	1041	CG2	VAL	295	72.783	37.993	29.101	1.00	23.07
ATOM	1042	C	VAL	295	75.057	38.062	25.993	1.00	33.92
ATOM	1043	O	VAL	295	74.932	37.238	25.090	1.00	36.95
ATOM	1044	N <sup>+</sup>	SER	296	75.625	39.253	25.820	1.00	31.27
ATOM	1045	CA	SER	296	76.118	39.695	24.521	1.00	33.38
ATOM	1046	CB	SER	296	76.667	41.115	24.620	1.00	24.78
ATOM	1047	OG	SER	296	77.368	41.478	23.449	1.00	25.43
ATOM	1048	C	SER	296	77.216	38.748	24.045	1.00	35.86
ATOM	1049	O	SER	296	77.220	38.324	22.886	1.00	39.60
ATOM	1050	N	ASP	297	78.135	38.402	24.943	1.00	37.41
ATOM	1051	CA	ASP	297	79.227	37.490	24.602	1.00	35.39
ATOM	1052	CB	ASP	297	80.147	37.269	25.808	1.00	43.07
ATOM	1053	CG	ASP	297	80.839	38.540	26.266	1.00	45.07
ATOM	1054	OD1	ASP	297	81.175	39.398	25.419	1.00	48.02
ATOM	1055	OD2	ASP	297	81.064	38.670	27.485	1.00	50.13
ATOM	1056	C	ASP	297	78.662	36.145	24.161	1.00	30.87
ATOM	1057	O	ASP	297	79.155	35.534	23.213	1.00	33.92
ATOM	1058	N	ALA	298	77.625	35.698	24.861	1.00	28.96
ATOM	1059	CA	ALA	298	76.971	34.428	24.574	1.00	30.60
ATOM	1060	CB	ALA	298	75.889	34.157	25.610	1.00	27.56
ATOM	1061	C	ALA	298	76.377	34.408	23.163	1.00	33.04
ATOM	1062	O	ALA	298	76.538	33.426	22.426	1.00	32.48
ATOM	1063	N	ILE	299	75.706	35.493	22.786	1.00	30.92
ATOM	1064	CA	ILE	299	75.091	35.588	21.468	1.00	24.71
ATOM	1065	CB	ILE	299	74.138	36.789	21.368	1.00	22.98
ATOM	1066	CG2	ILE	299	73.430	36.786	20.018	1.00	21.90
ATOM	1067	CG1	ILE	299	73.091	36.707	22.477	1.00	20.91
ATOM	1068	CD1	ILE	299	72.266	37.951	22.634	1.00	19.86
ATOM	1069	C	ILE	299	76.168	35.680	20.395	1.00	26.77
ATOM	1070	O	ILE	299	76.036	35.069	19.335	1.00	30.21
ATOM	1071	N	PHE	300	77.238	36.428	20.673	1.00	29.08
ATOM	1072	CA	PHE	300	78.345	36.562	19.726	1.00	28.06
ATOM	1073	CB	PHE	300	79.386	37.565	20.235	1.00	29.06
ATOM	1074	CG	PHE	300	79.289	38.920	19.590	1.00	28.14
ATOM	1075	CD1	PHE	300	78.449	39.896	20.113	1.00	27.20
ATOM	1076	CD2	PHE	300	80.017	39.209	18.437	1.00	29.11
ATOM	1077	CE1	PHE	300	78.332	41.139	19.499	1.00	28.18
ATOM	1078	CE2	PHE	300	79.908	40.450	17.815	1.00	29.07
ATOM	1079	CZ	PHE	300	79.064	41.416	18.348	1.00	22.61
ATOM	1080	C	PHE	300	78.991	35.201	19.485	1.00	29.00
ATOM	1081	O	PHE	300	79.278	34.833	18.344	1.00	30.35
ATOM	1082	N	GLU	301	79.183	34.442	20.560	1.00	31.81
ATOM	1083	CA	GLU	301	79.767	33.111	20.470	1.00	34.96

ATOM	1086	O	GLU	301	79.322	31.438	18.793	1.00	35.76
ATOM	1087	N	LEU	302	77.543	32.313	19.869	1.00	32.14
ATOM	1088	CA	LEU	302	76.559	31.522	19.132	1.00	25.56
ATOM	1089	CB	LEU	302	75.147	31.760	19.682	1.00	23.33
ATOM	1090	CG	LEU	302	73.992	31.006	19.010	1.00	28.73
ATOM	1091	CD1	LEU	302	74.093	29.509	19.270	1.00	23.93
ATOM	1092	CD2	LEU	302	72.667	31.551	19.514	1.00	21.32
ATOM	1093	C	LEU	302	76.617	31.885	17.650	1.00	23.10
ATOM	1094	O	LEU	302	76.664	31.001	16.796	1.00	26.79
ATOM	1095	N	GLY	303	76.672	33.181	17.353	1.00	22.79
ATOM	1096	CA	GLY	303	76.745	33.631	15.974	1.00	21.60
ATOM	1097	C	GLY	303	77.978	33.104	15.256	1.00	30.42
ATOM	1098	O	GLY	303	77.889	32.619	14.125	1.00	29.18
ATOM	1099	N	ALA	304	79.132	33.182	15.912	1.00	31.15
ATOM	1100	CA	ALA	304	80.375	32.703	15.313	1.00	35.44
ATOM	1101	CB	ALA	304	81.562	32.995	16.235	1.00	29.16
ATOM	1102	C	ALA	304	80.300	31.208	14.978	1.00	35.15
ATOM	1103	O	ALA	304	80.705	30.785	13.891	1.00	37.13
ATOM	1104	N	SER	305	79.753	30.414	15.892	1.00	33.91
ATOM	1105	CA	SER	305	79.638	28.979	15.663	1.00	36.39
ATOM	1106	CB	SER	305	79.395	28.237	16.980	1.00	32.71
ATOM	1107	OG	SER	305	78.265	28.749	17.663	1.00	48.66
ATOM	1108	C	SER	305	78.558	28.619	14.641	1.00	37.61
ATOM	1109	O	SER	305	78.747	27.697	13.845	1.00	39.92
ATOM	1110	N	LEU	306	77.443	29.349	14.651	1.00	38.21
ATOM	1111	CA	LEU	306	76.350	29.092	13.714	1.00	35.65
ATOM	1112	CB	LEU	306	75.094	29.894	14.077	1.00	25.49
ATOM	1113	CG	LEU	306	74.209	29.374	15.212	1.00	26.18
ATOM	1114	CD1	LEU	306	72.988	30.262	15.361	1.00	23.40
ATOM	1115	CD2	LEU	306	73.777	27.952	14.921	1.00	23.57
ATOM	1116	C	LEU	306	76.723	29.356	12.258	1.00	38.05
ATOM	1117	O	LEU	306	76.092	28.809	11.353	1.00	37.22
ATOM	1118	N	SER	307	77.743	30.185	12.030	1.00	40.41
ATOM	1119	CA	SER	307	78.199	30.511	10.677	1.00	40.85
ATOM	1120	CB	SER	307	79.415	31.442	10.736	1.00	37.32
ATOM	1121	OG	SER	307	79.086	32.678	11.344	1.00	56.20
ATOM	1122	C	SER	307	78.550	29.270	9.852	1.00	39.87
ATOM	1123	O	SER	307	78.221	29.191	8.670	1.00	44.27
ATOM	1124	N	ALA	308	79.207	28.305	10.487	1.00	39.29
ATOM	1125	CA	ALA	308	79.609	27.066	9.826	1.00	33.10
ATOM	1126	CB	ALA	308	80.607	26.310	10.696	1.00	33.37
ATOM	1127	C	ALA	308	78.403	26.177	9.502	1.00	34.07
ATOM	1128	O	ALA	308	78.467	25.340	8.600	1.00	40.61
ATOM	1129	N	PHE	309	77.305	26.368	10.230	1.00	31.85
ATOM	1130	CA	PHE	309	76.095	25.581	10.015	1.00	35.24



ATOM	1133	CD1 PHE	309	76.785	25.327	13.090	1.00	43.79
ATOM	1134	CD2 PHE	309	74.903	23.867	12.922	1.00	38.03
ATOM	1135	CE1 PHE	309	77.237	24.627	14.210	1.00	41.12
ATOM	1136	CE2 PHE	309	75.346	23.161	14.040	1.00	41.08
ATOM	1137	CZ PHE	309	76.514	23.543	14.683	1.00	38.37
ATOM	1138	C' PHE	309	75.361	25.934	8.720	1.00	36.31
ATOM	1139	O PHE	309	74.633	25.095	8.173	1.00	37.84
ATOM	1140	N ASN	310	75.567	27.155	8.225	1.00	35.22
ATOM	1141	CA ASN	310	74.933	27.625	6.988	1.00	43.66
ATOM	1142	CB ASN	310	75.536	26.930	5.760	1.00	54.13
ATOM	1143	CG ASN	310	76.980	27.339	5.501	1.00	68.29
ATOM	1144	OD1 ASN	310	77.297	28.527	5.412	1.00	74.62
ATOM	1145	ND2 ASN	310	77.859	26.348	5.352	1.00	68.85
ATOM	1146	C ASN	310	73.430	27.385	7.013	1.00	38.37
ATOM	1147	O ASN	310	72.882	26.735	6.123	1.00	36.70
ATOM	1148	N LEU	311	72.780	27.865	8.062	1.00	35.22
ATOM	1149	CA LEU	311	71.345	27.690	8.206	1.00	34.32
ATOM	1150	CB LEU	311	70.895	28.054	9.630	1.00	30.19
ATOM	1151	CG LEU	311	71.458	27.306	10.845	1.00	26.76
ATOM	1152	CD1 LEU	311	70.792	27.847	12.104	1.00	21.37
ATOM	1153	CD2 LEU	311	71.217	25.813	10.722	1.00	22.95
ATOM	1154	C LEU	311	70.601	28.561	7.206	1.00	34.64
ATOM	1155	O LEU	311	71.087	29.625	6.820	1.00	37.70
ATOM	1156	N ASP	312	69.444	28.091	6.752	1.00	29.40
ATOM	1157	CA ASP	312	68.634	28.867	5.823	1.00	28.65
ATOM	1158	CB ASP	312	68.302	28.061	4.545	1.00	24.79
ATOM	1159	CG ASP	312	67.459	26.804	4.804	1.00	21.47
ATOM	1160	OD1 ASP	312	66.994	26.549	5.932	1.00	27.92
ATOM	1161	OD2 ASP	312	67.250	26.057	3.832	1.00	27.53
ATOM	1162	C ASP	312	67.380	29.346	6.557	1.00	25.92
ATOM	1163	O ASP	312	67.167	28.985	7.717	1.00	26.98
ATOM	1164	N ASP	313	66.540	30.122	5.878	1.00	21.78
ATOM	1165	CA ASP	313	65.315	30.653	6.471	1.00	22.89
ATOM	1166	CB ASP	313	64.517	31.458	5.439	1.00	29.19
ATOM	1167	CG ASP	313	65.216	32.739	5.025	1.00	36.82
ATOM	1168	OD1 ASP	313	65.985	33.285	5.845	1.00	41.51
ATOM	1169	OD2 ASP	313	64.997	33.203	3.883	1.00	44.19
ATOM	1170	C ASP	313	64.421	29.587	7.085	1.00	25.09
ATOM	1171	O ASP	313	63.778	29.829	8.110	1.00	27.60
ATOM	1172	N THR	314	64.363	28.420	6.449	1.00	20.90
ATOM	1173	CA THR	314	63.538	27.322	6.942	1.00	22.71
ATOM	1174	CB THR	314	63.408	26.208	5.884	1.00	22.07
ATOM	1175	OG1 THR	314	62.825	26.746	4.693	1.00	23.15
ATOM	1176	CG2 THR	314	62.542	25.079	6.401	1.00	18.17
ATOM	1177	C THR	314	64.080	26.734	8.249	1.00	19.95
ATOM	1178	O THR	314	63.326	26.477	9.182	1.00	22.40
ATOM	1179	N GLU	315	65.391	26.536	8.318	1.00	20.01



ATOM	1180	CA	GLU	315	65.997	25.987	9.523	1.00	19.40
ATOM	1181	CB	GLU	315	67.454	25.626	9.254	1.00	11.72
ATOM	1182	CG	GLU	315	67.544	24.440	8.322	1.00	13.43
ATOM	1183	CD	GLU	315	68.925	24.157	7.791	1.00	18.51
ATOM	1184	OE1	GLU	315	69.666	25.107	7.451	1.00	23.24
ATOM	1185	OE2	GLU	315	69.254	22.962	7.673	1.00	24.23
ATOM	1186	C	GLU	315	65.833	26.960	10.681	1.00	20.12
ATOM	1187	O	GLU	315	65.425	26.570	11.777	1.00	20.53
ATOM	1188	N	VAL	316	66.055	28.240	10.406	1.00	21.79
ATOM	1189	CA	VAL	316	65.898	29.270	11.425	1.00	18.14
ATOM	1190	CB	VAL	316	66.346	30.659	10.898	1.00	18.97
ATOM	1191	CG1	VAL	316	66.040	31.741	11.929	1.00	19.08
ATOM	1192	CG2	VAL	316	67.840	30.641	10.537	1.00	17.97
ATOM	1193	C	VAL	316	64.430	29.332	11.880	1.00	22.54
ATOM	1194	O	VAL	316	64.146	29.433	13.072	1.00	26.47
ATOM	1195	N	ALA	317	63.505	29.242	10.924	1.00	19.66
ATOM	1196	CA	ALA	317	62.076	29.286	11.216	1.00	16.99
ATOM	1197	CB	ALA	317	61.279	29.329	9.926	1.00	17.79
ATOM	1198	C	ALA	317	61.619	28.105	12.063	1.00	14.12
ATOM	1199	O	ALA	317	60.808	28.263	12.970	1.00	17.04
ATOM	1200	N	LEU	318	62.104	26.911	11.740	1.00	20.37
ATOM	1201	CA	LEU	318	61.725	25.714	12.485	1.00	21.12
ATOM	1202	CB	LEU	318	62.131	24.448	11.718	1.00	21.80
ATOM	1203	CG	LEU	318	61.364	24.265	10.398	1.00	18.11
ATOM	1204	CD1	LEU	318	61.946	23.125	9.594	1.00	16.79
ATOM	1205	CD2	LEU	318	59.891	24.024	10.676	1.00	12.66
ATOM	1206	C	LEU	318	62.335	25.752	13.880	1.00	22.03
ATOM	1207	O	LEU	318	61.688	25.373	14.858	1.00	21.35
ATOM	1208	N	LEU	319	63.564	26.257	13.964	1.00	20.03
ATOM	1209	CA	LEU	319	64.260	26.395	15.236	1.00	20.24
ATOM	1210	CB	LEU	319	65.657	26.960	15.001	1.00	19.07
ATOM	1211	CG	LEU	319	66.594	27.108	16.196	1.00	27.61
ATOM	1212	CD1	LEU	319	66.518	25.883	17.083	1.00	29.73
ATOM	1213	CD2	LEU	319	68.012	27.326	15.699	1.00	20.98
ATOM	1214	C	LEU	319	63.422	27.334	16.118	1.00	21.16
ATOM	1215	O	LEU	319	63.144	27.032	17.279	1.00	26.65
ATOM	1216	N	GLN	320	62.958	28.439	15.539	1.00	20.77
ATOM	1217	CA	GLN	320	62.119	29.390	16.265	1.00	17.87
ATOM	1218	CB	GLN	320	61.781	30.594	15.388	1.00	18.74
ATOM	1219	CG	GLN	320	62.957	31.496	15.111	1.00	21.07
ATOM	1220	CD	GLN	320	62.637	32.617	14.150	1.00	22.88
ATOM	1221	OE1	GLN	320	61.571	32.653	13.528	1.00	26.07
ATOM	1222	NE2	GLN	320	63.574	33.537	14.006	1.00	20.11
ATOM	1223	C	GLN	320	60.829	28.728	16.730	1.00	19.08
ATOM	1224	O	GLN	320	60.368	28.976	17.844		

ATOM	1227	CB	ALA	321	58.495	26.422	14.993	1.00	17.22
ATOM	1228	C	ALA	321	59.220	26.235	17.376	1.00	19.85
ATOM	1229	O	ALA	321	58.362	26.119	18.250	1.00	19.60
ATOM	1230	N	VAL	322	60.368	25.561	17.396	1.00	20.25
ATOM	1231	CA	VAL	322	60.693	24.628	18.469	1.00	21.32
ATOM	1232	CB	VAL	322	61.956	23.800	18.116	1.00	20.46
ATOM	1233	CG1	VAL	322	62.418	22.971	19.304	1.00	20.39
ATOM	1234	CG2	VAL	322	61.662	22.890	16.930	1.00	16.83
ATOM	1235	C	VAL	322	60.880	25.393	19.785	1.00	20.67
ATOM	1236	O	VAL	322	60.444	24.941	20.850	1.00	21.28
ATOM	1237	N	LEU	323	61.492	26.574	19.701	1.00	21.14
ATOM	1238	CA	LEU	323	61.722	27.417	20.869	1.00	22.94
ATOM	1239	CB	LEU	323	62.610	28.608	20.511	1.00	16.12
ATOM	1240	CG	LEU	323	64.051	28.291	20.115	1.00	22.28
ATOM	1241	CD1	LEU	323	64.719	29.532	19.528	1.00	14.87
ATOM	1242	CD2	LEU	323	64.816	27.750	21.320	1.00	21.55
ATOM	1243	C	LEU	323	60.398	27.932	21.410	1.00	22.55
ATOM	1244	O	LEU	323	60.185	27.986	22.615	1.00	25.21
ATOM	1245	N	LEU	324	59.507	28.300	20.502	1.00	24.15
ATOM	1246	CA	LEU	324	58.200	28.827	20.855	1.00	19.88
ATOM	1247	CB	LEU	324	57.499	29.384	19.608	1.00	15.20
ATOM	1248	CG	LEU	324	56.067	29.908	19.767	1.00	17.21
ATOM	1249	CD1	LEU	324	56.021	31.161	20.637	1.00	15.99
ATOM	1250	CD2	LEU	324	55.496	30.208	18.395	1.00	20.03
ATOM	1251	C	LEU	324	57.311	27.795	21.536	1.00	19.83
ATOM	1252	O	LEU	324	56.767	28.064	22.609	1.00	24.47
ATOM	1253	N	MET	325	57.197	26.603	20.956	1.00	25.02
ATOM	1254	CA	MET	325	56.339	25.563	21.522	1.00	26.72
ATOM	1255	CB	MET	325	55.823	24.644	20.410	1.00	30.03
ATOM	1256	CG	MET	325	55.129	25.358	19.241	1.00	25.09
ATOM	1257	SD	MET	325	53.714	26.409	19.672	1.00	27.29
ATOM	1258	CE	MET	325	52.503	25.220	20.084	1.00	20.67
ATOM	1259	C	MET	325	56.995	24.736	22.635	1.00	28.94
ATOM	1260	O	MET	325	56.881	23.510	22.672	1.00	32.94
ATOM	1261	N	SER	326	57.642	25.418	23.569	1.00	29.36
ATOM	1262	CA	SER	326	58.311	24.759	24.680	1.00	31.62
ATOM	1263	CB	SER	326	59.554	25.559	25.064	1.00	38.13
ATOM	1264	OG	SER	326	60.277	24.949	26.119	1.00	48.99
ATOM	1265	C	SER	326	57.361	24.653	25.871	1.00	33.69
ATOM	1266	O	SER	326	56.620	25.594	26.166	1.00	33.66
ATOM	1267	N	THR	327	57.356	23.499	26.536	1.00	38.27
ATOM	1268	CA	THR	327	56.497	23.306	27.701	1.00	38.98
ATOM	1269	CB	THR	327	55.875	21.896	27.730	1.00	33.30
ATOM	1270	OG1	THR	327	56.908	20.911	27.627	1.00	44.01
ATOM	1271	CG2	THR	327	54.888	21.722	26.587	1.00	38.

ATOM	1274	N	ASP	328	58.462	24.091	28.924	1.00	45.92
ATOM	1275	CA	ASP	328	59.268	24.410	30.104	1.00	49.59
ATOM	1276	CB	ASP	328	60.760	24.411	29.760	1.00	59.87
ATOM	1277	CG	ASP	328	61.273	23.040	29.387	1.00	75.73
ATOM	1278	OD1	ASP	328	62.008	22.939	28.382	1.00	85.81
ATOM	1279	OD2	ASP	328	60.946	22.063	30.098	1.00	85.56
ATOM	1280	C	ASP	328	58.873	25.767	30.673	1.00	48.50
ATOM	1281	O	ASP	328	59.725	26.609	30.961	1.00	57.50
ATOM	1282	N	ARG	329	57.569	25.980	30.805	1.00	49.62
ATOM	1283	CA	ARG	329	57.032	27.222	31.340	1.00	50.52
ATOM	1284	CB	ARG	329	56.400	28.080	30.230	1.00	53.57
ATOM	1285	CG	ARG	329	57.376	28.828	29.324	1.00	51.09
ATOM	1286	CD	ARG	329	57.897	27.951	28.204	1.00	49.73
ATOM	1287	NE	ARG	329	58.692	28.699	27.233	1.00	47.44
ATOM	1288	CZ	ARG	329	60.005	28.569	27.080	1.00	54.28
ATOM	1289	NH1	ARG	329	60.688	27.722	27.839	1.00	58.35
ATOM	1290	NH2	ARG	329	60.631	29.256	26.136	1.00	51.92
ATOM	1291	C	ARG	329	55.970	26.870	32.375	1.00	51.90
ATOM	1292	O	ARG	329	55.378	25.790	32.324	1.00	50.77
ATOM	1293	N	SER	330	55.728	27.784	33.303	1.00	50.56
ATOM	1294	CA	SER	330	54.744	27.564	34.349	1.00	50.67
ATOM	1295	CB	SER	330	55.271	28.108	35.678	1.00	46.64
ATOM	1296	C	SER	330	53.404	28.213	34.004	1.00	47.63
ATOM	1297	O	SER	330	53.371	29.309	33.440	1.00	48.02
ATOM	1298	N	GLY	331	52.314	27.496	34.277	1.00	44.44
ATOM	1299	CA	GLY	331	50.977	28.023	34.044	1.00	38.77
ATOM	1300	C	GLY	331	50.236	27.710	32.756	1.00	41.74
ATOM	1301	O	GLY	331	49.147	28.246	32.537	1.00	49.57
ATOM	1302	N	LEU	332	50.783	26.841	31.912	1.00	39.75
ATOM	1303	CA	LEU	332	50.123	26.502	30.651	1.00	37.55
ATOM	1304	CB	LEU	332	51.107	25.829	29.694	1.00	32.36
ATOM	1305	CG	LEU	332	52.268	26.659	29.153	1.00	34.40
ATOM	1306	CD1	LEU	332	53.207	25.749	28.379	1.00	30.22
ATOM	1307	CD2	LEU	332	51.742	27.786	28.277	1.00	23.33
ATOM	1308	C	LEU	332	48.921	25.589	30.834	1.00	36.73
ATOM	1309	O	LEU	332	48.987	24.608	31.577	1.00	39.29
ATOM	1310	N	LEU	333	47.822	25.925	30.168	1.00	36.07
ATOM	1311	CA	LEU	333	46.615	25.107	30.215	1.00	39.58
ATOM	1312	CB	LEU	333	45.384	25.906	29.754	1.00	41.08
ATOM	1313	CG	LEU	333	44.601	26.883	30.644	1.00	47.59
ATOM	1314	CD1	LEU	333	44.268	26.213	31.961	1.00	45.65
ATOM	1315	CD2	LEU	333	45.366	28.171	30.874	1.00	47.42
ATOM	1316	C	LEU	333	46.791	23.911	29.278	1.00	40.00
ATOM	1317	O	LEU	333	46.690	22.754	29.689	1.00	44.77
ATOM	1318	N	CYA	334	47.102	24.213	28.022	1.00	

ATOM	1321	SG	CYA	334	45.280	24.738	25.758	1.00	44.31
ATOM	1322	AS	CYA	334	43.972	22.946	25.380	1.00	76.30
ATOM	1323	C	CYA	334	48.668	22.617	26.815	1.00	34.91
ATOM	1324	O	CYA	334	49.237	22.615	25.722	1.00	37.63
ATOM	1325	N	VAL	335	49.189	22.056	27.903	1.00	35.43
ATOM	1326	CA	VAL	335	50.518	21.452	27.909	1.00	34.27
ATOM	1327	CB	VAL	335	50.861	20.868	29.298	1.00	34.21
ATOM	1328	CG1	VAL	335	52.261	20.258	29.292	1.00	33.66
ATOM	1329	CG2	VAL	335	50.755	21.945	30.362	1.00	31.77
ATOM	1330	C	VAL	335	50.662	20.349	26.865	1.00	37.14
ATOM	1331	O	VAL	335	51.639	20.320	26.114	1.00	37.59
ATOM	1332	N	ASP	336	49.683	19.451	26.813	1.00	39.99
ATOM	1333	CA	ASP	336	49.705	18.339	25.866	1.00	41.64
ATOM	1334	CB	ASP	336	48.532	17.392	26.146	1.00	54.27
ATOM	1335	CG	ASP	336	48.596	16.118	25.322	1.00	67.42
ATOM	1336	OD1	ASP	336	47.915	16.049	24.274	1.00	70.98
ATOM	1337	OD2	ASP	336	49.337	15.191	25.717	1.00	76.88
ATOM	1338	C	ASP	336	49.702	18.762	24.393	1.00	38.31
ATOM	1339	O	ASP	336	50.469	18.229	23.586	1.00	37.46
ATOM	1340	N	LYS	337	48.853	19.729	24.052	1.00	30.23
ATOM	1341	CA	LYS	337	48.740	20.211	22.676	1.00	29.21
ATOM	1342	CB	LYS	337	47.561	21.189	22.559	1.00	30.53
ATOM	1343	CG	LYS	337	47.012	21.360	21.162	1.00	51.63
ATOM	1344	CD	LYS	337	45.636	21.997	21.186	1.00	59.57
ATOM	1345	CE	LYS	337	45.066	22.115	19.774	1.00	66.05
ATOM	1346	NZ	LYS	337	43.673	22.693	19.776	1.00	67.20
ATOM	1347	C	LYS	337	50.054	20.873	22.249	1.00	28.33
ATOM	1348	O	LYS	337	50.581	20.594	21.170	1.00	26.08
ATOM	1349	N	ILE	338	50.609	21.696	23.141	1.00	26.74
ATOM	1350	CA	ILE	338	51.873	22.390	22.902	1.00	25.42
ATOM	1351	CB	ILE	338	52.177	23.379	24.052	1.00	23.57
ATOM	1352	CG2	ILE	338	53.559	23.991	23.874	1.00	22.59
ATOM	1353	CG1	ILE	338	51.105	24.471	24.096	1.00	23.57
ATOM	1354	CD1	ILE	338	51.157	25.362	25.333	1.00	24.30
ATOM	1355	C	ILE	338	53.018	21.382	22.768	1.00	29.20
ATOM	1356	O	ILE	338	53.905	21.537	21.916	1.00	31.59
ATOM	1357	N	GLU	339	52.977	20.340	23.595	1.00	34.82
ATOM	1358	CA	GLU	339	53.980	19.277	23.597	1.00	34.23
ATOM	1359	CB	GLU	339	53.639	18.256	24.681	1.00	40.38
ATOM	1360	CG	GLU	339	54.785	17.354	25.072	1.00	54.98
ATOM	1361	CD	GLU	339	55.644	17.964	26.178	1.00	71.26
ATOM	1362	OE1	GLU	339	56.766	18.444	25.858	1.00	77.82
ATOM	1363	OE2	GLU	339	55.170	17.985	27.349	1.00	65.14
ATOM	1364	C	GLU	339	53.972	18.582	22.231	1.00	34.42
ATOM	1365	O	GLU	339	55.018	18.431	21.590	1.00	



ATOM	1368	CB	LYS	340	51.121	17.105	20.325	1.00	34.59
ATOM	1369	C	LYS	340	53.064	18.390	19.337	1.00	32.56
ATOM	1370	O	LYS	340	53.762	17.913	18.441	1.00	32.93
ATOM	1371	N	SER	341	52.725	19.677	19.374	1.00	31.42
ATOM	1372	CA	SER	341	53.134	20.621	18.334	1.00	27.79
ATOM	1373	CB	SER	341	52.559	22.009	18.601	1.00	27.85
ATOM	1374	OG	SER	341	51.149	21.966	18.579	1.00	47.20
ATOM	1375	C	SER	341	54.647	20.713	18.240	1.00	26.01
ATOM	1376	O	SER	341	55.205	20.706	17.139	1.00	27.10
ATOM	1377	N	GLN	342	55.318	20.794	19.389	1.00	24.25
ATOM	1378	CA	GLN	342	56.771	20.875	19.392	1.00	27.16
ATOM	1379	CB	GLN	342	57.309	21.089	20.799	1.00	25.60
ATOM	1380	CG	GLN	342	58.768	21.466	20.777	1.00	27.99
ATOM	1381	CD	GLN	342	59.407	21.429	22.133	1.00	29.58
ATOM	1382	OE1	GLN	342	60.123	22.356	22.513	1.00	31.18
ATOM	1383	NE2	GLN	342	59.184	20.345	22.868	1.00	29.17
ATOM	1384	C	GLN	342	57.377	19.609	18.786	1.00	28.45
ATOM	1385	O	GLN	342	58.378	19.675	18.062	1.00	29.79
ATOM	1386	N	GLU	343	56.777	18.458	19.078	1.00	26.58
ATOM	1387	CA	GLU	343	57.251	17.190	18.525	1.00	30.07
ATOM	1388	CB	GLU	343	56.462	16.016	19.114	1.00	40.79
ATOM	1389	CG	GLU	343	56.812	15.700	20.568	1.00	61.22
ATOM	1390	CD	GLU	343	55.951	14.594	21.166	1.00	71.76
ATOM	1391	OE1	GLU	343	55.472	13.719	20.405	1.00	76.73
ATOM	1392	OE2	GLU	343	55.758	14.601	22.403	1.00	74.09
ATOM	1393	C	GLU	343	57.097	17.225	17.001	1.00	25.87
ATOM	1394	O	GLU	343	58.008	16.842	16.260	1.00	27.26
ATOM	1395	N	ALA	344	55.947	17.727	16.550	1.00	23.70
ATOM	1396	CA	ALA	344	55.647	17.853	15.124	1.00	22.16
ATOM	1397	CB	ALA	344	54.275	18.489	14.927	1.00	21.18
ATOM	1398	C	ALA	344	56.729	18.694	14.454	1.00	21.24
ATOM	1399	O	ALA	344	57.303	18.284	13.438	1.00	26.47
ATOM	1400	N	TYR	345	57.048	19.840	15.055	1.00	22.48
ATOM	1401	CA	TYR	345	58.073	20.738	14.531	1.00	21.41
ATOM	1402	CB	TYR	345	58.085	22.059	15.304	1.00	20.10
ATOM	1403	CG	TYR	345	57.023	23.015	14.830	1.00	15.87
ATOM	1404	CD1	TYR	345	56.004	23.434	15.682	1.00	10.54
ATOM	1405	CE1	TYR	345	54.983	24.259	15.225	1.00	17.09
ATOM	1406	CD2	TYR	345	57.003	23.448	13.505	1.00	16.86
ATOM	1407	CE2	TYR	345	55.991	24.269	13.036	1.00	16.84
ATOM	1408	CZ	TYR	345	54.984	24.668	13.896	1.00	17.97
ATOM	1409	OH	TYR	345	53.963	25.455	13.406	1.00	27.11
ATOM	1410	C	TYR	345	59.465	20.120	14.548	1.00	24.43
ATOM	1411	O	TYR	345	60.238	20.291	13.597	1.00	24.69
ATOM	1412	N	LEU	346	59.777	19.401	15.62		



ATOM	1415	CG	LEU	346	61.637	19.076	18.252	1.00	26.46
ATOM	1416	CD1	LEU	346	61.387	18.468	19.610	1.00	26.46
ATOM	1417	CD2	LEU	346	63.101	19.437	18.076	1.00	21.78
ATOM	1418	C	LEU	346	61.322	17.713	14.683	1.00	23.24
ATOM	1419	O	LEU	346	62.416	17.645	14.127	1.00	27.54
ATOM	1420	N	LEU	347	60.314	16.900	14.395	1.00	25.75
ATOM	1421	CA	LEU	347	60.437	15.881	13.356	1.00	25.41
ATOM	1422	CB	LEU	347	59.208	14.970	13.330	1.00	23.78
ATOM	1423	CG	LEU	347	59.302	13.713	14.190	1.00	31.85
ATOM	1424	CD1	LEU	347	58.004	12.928	14.089	1.00	39.88
ATOM	1425	CD2	LEU	347	60.483	12.864	13.738	1.00	27.65
ATOM	1426	C	LEU	347	60.611	16.535	11.998	1.00	23.22
ATOM	1427	O	LEU	347	61.468	16.133	11.211	1.00	28.58
ATOM	1428	N	ALA	348	59.784	17.542	11.731	1.00	26.40
ATOM	1429	CA	ALA	348	59.840	18.273	10.474	1.00	23.85
ATOM	1430	CB	ALA	348	58.732	19.324	10.433	1.00	25.27
ATOM	1431	C	ALA	348	61.210	18.924	10.337	1.00	23.69
ATOM	1432	O	ALA	348	61.847	18.835	9.288	1.00	29.11
ATOM	1433	N	PHE	349	61.678	19.506	11.438	1.00	24.71
ATOM	1434	CA	PHE	349	62.973	20.181	11.493	1.00	20.48
ATOM	1435	CB	PHE	349	63.164	20.772	12.900	1.00	17.84
ATOM	1436	CG	PHE	349	64.334	21.721	13.031	1.00	14.90
ATOM	1437	CD1	PHE	349	65.109	22.069	11.933	1.00	17.58
ATOM	1438	CD2	PHE	349	64.651	22.269	14.271	1.00	24.77
ATOM	1439	CE1	PHE	349	66.185	22.944	12.063	1.00	20.26
ATOM	1440	CE2	PHE	349	65.727	23.147	14.413	1.00	23.83
ATOM	1441	CZ	PHE	349	66.494	23.486	13.299	1.00	20.36
ATOM	1442	C	PHE	349	64.084	19.181	11.159	1.00	23.43
ATOM	1443	O	PHE	349	64.916	19.427	10.278	1.00	24.35
ATOM	1444	N	GLU	350	64.057	18.028	11.820	1.00	25.79
ATOM	1445	CA	GLU	350	65.060	16.991	11.606	1.00	26.75
ATOM	1446	CB	GLU	350	64.813	15.822	12.567	1.00	29.56
ATOM	1447	CG	GLU	350	65.774	14.661	12.391	1.00	39.94
ATOM	1448	CD	GLU	350	65.574	13.549	13.407	1.00	45.06
ATOM	1449	OE1	GLU	350	64.413	13.192	13.715	1.00	49.26
ATOM	1450	OE2	GLU	350	66.593	13.017	13.887	1.00	56.67
ATOM	1451	C	GLU	350	65.051	16.494	10.162	1.00	26.95
ATOM	1452	O	GLU	350	66.096	16.398	9.513	1.00	28.77
ATOM	1453	N	HIS	351	63.858	16.219	9.652	1.00	22.56
ATOM	1454	CA	HIS	351	63.699	15.728	8.294	1.00	22.20
ATOM	1455	CB	HIS	351	62.263	15.265	8.083	1.00	22.47
ATOM	1456	CG	HIS	351	61.881	14.106	8.947	1.00	23.61
ATOM	1457	CD2	HIS	351	62.633	13.300	9.739	1.00	27.65
ATOM	1458	ND1	HIS	351	60.585	13.653	9.069	1.00	26.13
ATOM	1459	CE1	HIS	351	60.548	12.629	9.898	1.00	

ATOM	1462	O	HIS	351	64.708	16.419	6.226	1.00	27.02
ATOM	1463	N	TYR	352	63.909	18.041	7.555	1.00	18.26
ATOM	1464	CA	TYR	352	64.327	19.101	6.649	1.00	16.94
ATOM	1465	CB	TYR	352	63.749	20.455	7.066	1.00	19.07
ATOM	1466	CG	TYR	352	64.107	21.534	6.081	1.00	21.11
ATOM	1467	CD1	TYR	352	63.518	21.564	4.819	1.00	21.33
ATOM	1468	CE1	TYR	352	63.921	22.482	3.859	1.00	21.06
ATOM	1469	CD2	TYR	352	65.105	22.462	6.367	1.00	22.07
ATOM	1470	CE2	TYR	352	65.515	23.388	5.412	1.00	25.40
ATOM	1471	CZ	TYR	352	64.921	23.384	4.161	1.00	21.90
ATOM	1472	OH	TYR	352	65.334	24.268	3.197	1.00	23.57
ATOM	1473	C	TYR	352	65.853	19.156	6.657	1.00	18.49
ATOM	1474	O	TYR	352	66.487	19.323	5.609	1.00	24.99
ATOM	1475	N	VAL	353	66.451	19.008	7.836	1.00	24.64
ATOM	1476	CA	VAL	353	67.904	19.011	7.955	1.00	22.20
ATOM	1477	CB	VAL	353	68.350	18.925	9.440	1.00	23.72
ATOM	1478	CG1	VAL	353	69.838	18.597	9.546	1.00	21.24
ATOM	1479	CG2	VAL	353	68.063	20.245	10.142	1.00	20.07
ATOM	1480	C	VAL	353	68.452	17.829	7.146	1.00	25.07
ATOM	1481	O	VAL	353	69.467	17.955	6.457	1.00	24.75
ATOM	1482	N	ASN	354	67.768	16.690	7.221	1.00	24.59
ATOM	1483	CA	ASN	354	68.171	15.502	6.474	1.00	25.64
ATOM	1484	CB	ASN	354	67.223	14.331	6.751	1.00	26.05
ATOM	1485	CG	ASN	354	67.368	13.763	8.151	1.00	30.27
ATOM	1486	OD1	ASN	354	66.443	13.139	8.672	1.00	33.71
ATOM	1487	ND2	ASN	354	68.529	13.959	8.765	1.00	34.78
ATOM	1488	C	ASN	354	68.143	15.813	4.981	1.00	30.50
ATOM	1489	O	ASN	354	69.042	15.423	4.233	1.00	33.73
ATOM	1490	N	HIS	355	67.098	16.519	4.555	1.00	30.54
ATOM	1491	CA	HIS	355	66.926	16.901	3.157	1.00	26.02
ATOM	1492	CB	HIS	355	65.535	17.521	2.953	1.00	29.93
ATOM	1493	CG	HIS	355	65.367	18.217	1.638	1.00	37.91
ATOM	1494	CD2	HIS	355	65.654	19.486	1.264	1.00	31.26
ATOM	1495	ND1	HIS	355	64.861	17.593	0.518	1.00	32.67
ATOM	1496	CE1	HIS	355	64.843	18.447	-0.488	1.00	33.22
ATOM	1497	NE2	HIS	355	65.322	19.601	-0.061	1.00	32.69
ATOM	1498	C	HIS	355	68.009	17.851	2.652	1.00	24.29
ATOM	1499	O	HIS	355	68.381	17.798	1.484	1.00	26.82
ATOM	1500	N	ARG	356	68.484	18.735	3.526	1.00	29.72
ATOM	1501	CA	ARG	356	69.516	19.711	3.167	1.00	26.65
ATOM	1502	CB	ARG	356	69.593	20.804	4.225	1.00	22.74
ATOM	1503	CG	ARG	356	68.409	21.735	4.222	1.00	21.64
ATOM	1504	CD	ARG	356	68.757	23.024	3.524	1.00	28.04
ATOM	1505	NE	ARG	356	69.550	23.900	4.380	1.00	33.79
ATOM	1506	CZ	ARG	356	70.508	24.716	3.952	1.00	29.26
ATOM	1507	NH1	ARG	3					

ATOM	1509	C	ARG	356	70.904	19.115	2.950	1.00	27.58
ATOM	1510	O	ARG	356	71.757	19.740	2.312	1.00	31.44
ATOM	1511	N	LYS	357	71.140	17.937	3.519	1.00	30.56
ATOM	1512	CA	LYS	357	72.422	17.244	3.390	1.00	34.56
ATOM	1513	CB	LYS	357	72.500	16.518	2.043	1.00	39.66
ATOM	1514	CG	LYS	357	71.476	15.402	1.871	1.00	42.16
ATOM	1515	CD	LYS	357	71.674	14.676	0.550	1.00	54.23
ATOM	1516	CE	LYS	357	70.691	13.523	0.371	1.00	61.97
ATOM	1517	NZ	LYS	357	69.288	13.974	0.162	1.00	65.88
ATOM	1518	C	LYS	357	73.665	18.119	3.606	1.00	36.73
ATOM	1519	O	LYS	357	74.522	18.248	2.728	1.00	40.70
ATOM	1520	N	HIS	358	73.738	18.732	4.786	1.00	33.69
ATOM	1521	CA	HIS	358	74.863	19.581	5.163	1.00	33.59
ATOM	1522	CB	HIS	358	74.660	20.155	6.571	1.00	32.07
ATOM	1523	CG	HIS	358	73.593	21.200	6.666	1.00	29.74
ATOM	1524	CD2	HIS	358	72.245	21.098	6.736	1.00	23.35
ATOM	1525	ND1	HIS	358	73.876	22.547	6.731	1.00	28.13
ATOM	1526	CE1	HIS	358	72.752	23.231	6.834	1.00	26.94
ATOM	1527	NE2	HIS	358	71.747	22.373	6.838	1.00	23.32
ATOM	1528	C	HIS	358	76.121	18.720	5.180	1.00	37.98
ATOM	1529	O	HIS	358	76.087	17.581	5.654	1.00	41.07
ATOM	1530	N	ASN	359	77.231	19.261	4.690	1.00	44.20
ATOM	1531	CA	ASN	359	78.492	18.523	4.676	1.00	49.72
ATOM	1532	CB	ASN	359	79.406	19.053	3.572	1.00	46.66
ATOM	1533	C	ASN	359	79.174	18.648	6.039	1.00	51.77
ATOM	1534	O	ASN	359	80.356	18.985	6.122	1.00	57.32
ATOM	1535	N	ILE	360	78.414	18.383	7.101	1.00	51.04
ATOM	1536	CA	ILE	360	78.906	18.471	8.477	1.00	48.24
ATOM	1537	CB	ILE	360	78.340	19.721	9.207	1.00	47.20
ATOM	1538	CG2	ILE	360	78.781	19.741	10.673	1.00	43.50
ATOM	1539	CG1	ILE	360	78.777	21.005	8.491	1.00	45.94
ATOM	1540	CD1	ILE	360	78.157	22.262	9.050	1.00	43.00
ATOM	1541	C	ILE	360	78.462	17.222	9.239	1.00	47.23
ATOM	1542	O	ILE	360	77.272	16.901	9.278	1.00	45.13
ATOM	1543	N	PRO	361	79.416	16.490	9.838	1.00	48.61
ATOM	1544	CD	PRO	361	80.869	16.705	9.729	1.00	50.93
ATOM	1545	CA	PRO	361	79.129	15.270	10.599	1.00	45.46
ATOM	1546	CB	PRO	361	80.524	14.725	10.927	1.00	49.01
ATOM	1547	CG	PRO	361	81.402	15.307	9.862	1.00	54.41
ATOM	1548	C	PRO	361	78.330	15.514	11.879	1.00	36.54
ATOM	1549	O	PRO	361	78.666	16.394	12.672	1.00	39.83
ATOM	1550	N	HIS	362	77.282	14.716	12.075	1.00	31.35
ATOM	1551	CA	HIS	362	76.430	14.798	13.264	1.00	33.34
ATOM	1552	CB	HIS	362	77.246	14.495	14.524	1.00	33.77
ATOM	1553	CG	HIS	362	78.129	13.292	14.397	1.00	34.40
ATOM	1554	CD2	HIS	362					

ATOM	1556	CE1 HIS	362	80.017	12.160	14.311	1.00	36.26
ATOM	1557	NE2 HIS	362	79.029	11.316	14.080	1.00	35.73
ATOM	1558	C HIS	362	75.778	16.164	13.389	1.00	33.55
ATOM	1559	O HIS	362	75.539	16.652	14.495	1.00	31.93
ATOM	1560	N PHE	363	75.449	16.748	12.240	1.00	35.83
ATOM	1561	CA PHE	363	74.834	18.067	12.166	1.00	30.93
ATOM	1562	CB PHE	363	74.464	18.394	10.712	1.00	28.82
ATOM	1563	CG PHE	363	73.959	19.797	10.514	1.00	26.59
ATOM	1564	CD1 PHE	363	74.846	20.843	10.301	1.00	26.96
ATOM	1565	CD2 PHE	363	72.596	20.076	10.575	1.00	27.51
ATOM	1566	CE1 PHE	363	74.384	22.151	10.155	1.00	31.83
ATOM	1567	CE2 PHE	363	72.124	21.378	10.433	1.00	26.65
ATOM	1568	CZ PHE	363	73.019	22.417	10.223	1.00	24.42
ATOM	1569	C PHE	363	73.613	18.235	13.063	1.00	28.73
ATOM	1570	O PHE	363	73.550	19.174	13.848	1.00	25.33
ATOM	1571	N TRP	364	72.663	17.310	12.969	1.00	22.89
ATOM	1572	CA TRP	364	71.443	17.405	13.760	1.00	24.19
ATOM	1573	CB TRP	364	70.481	16.254	13.439	1.00	26.31
ATOM	1574	CG TRP	364	69.198	16.275	14.228	1.00	20.24
ATOM	1575	CD2 TRP	364	68.213	17.325	14.262	1.00	24.50
ATOM	1576	CE2 TRP	364	67.175	16.894	15.120	1.00	25.84
ATOM	1577	CE3 TRP	364	68.106	18.583	13.652	1.00	25.83
ATOM	1578	CD1 TRP	364	68.731	15.289	15.040	1.00	23.61
ATOM	1579	NE1 TRP	364	67.515	15.648	15.579	1.00	32.26
ATOM	1580	CZ2 TRP	364	66.048	17.674	15.386	1.00	21.95
ATOM	1581	CZ3 TRP	364	66.979	19.360	13.919	1.00	20.73
ATOM	1582	CH2 TRP	364	65.967	18.899	14.779	1.00	22.37
ATOM	1583	C TRP	364	71.663	17.551	15.267	1.00	28.84
ATOM	1584	O TRP	364	71.246	18.554	15.839	1.00	31.25
ATOM	1585	N PRO	365	72.305	16.568	15.932	1.00	29.69
ATOM	1586	CD PRO	365	72.790	15.245	15.497	1.00	30.89
ATOM	1587	CA PRO	365	72.499	16.748	17.373	1.00	25.62
ATOM	1588	CB PRO	365	73.195	15.451	17.810	1.00	25.50
ATOM	1589	CG PRO	365	73.804	14.915	16.560	1.00	34.15
ATOM	1590	C PRO	365	73.320	18.002	17.698	1.00	24.07
ATOM	1591	O PRO	365	73.079	18.654	18.711	1.00	23.58
ATOM	1592	N LYS	366	74.250	18.365	16.820	1.00	24.09
ATOM	1593	CA LYS	366	75.063	19.562	17.027	1.00	29.44
ATOM	1594	CB LYS	366	76.131	19.681	15.945	1.00	27.18
ATOM	1595	CG LYS	366	77.341	18.802	16.149	1.00	23.71
ATOM	1596	CD LYS	366	78.304	19.019	15.001	1.00	27.50
ATOM	1597	CE LYS	366	79.624	18.329	15.231	1.00	35.88
ATOM	1598	NZ LYS	366	80.550	18.591	14.097	1.00	41.92
ATOM	1599	C LYS	366	74.195	20.820	17.012	1.00	32.76
ATOM	1600	O LYS	366	74.326	21.694	17.873	1.00	36.13
ATOM	1601	N LEU	367	73.307	20.907	16.028	1.00	33.70
ATOM	1602	CA LEU	367	72.409	22.041	15.905	1.00	30.60



ATOM	1603	CB	LEU	367	71.636	21.955	14.587	1.00	24.26
ATOM	1604	CG	LEU	367	70.675	23.103	14.274	1.00	32.42
ATOM	1605	CD1	LEU	367	71.394	24.440	14.404	1.00	24.78
ATOM	1606	CD2	LEU	367	70.098	22.924	12.878	1.00	28.84
ATOM	1607	C	LEU	367	71.450	22.015	17.087	1.00	31.90
ATOM	1608	O <sup>-</sup>	LEU	367	71.113	23.052	17.655	1.00	39.20
ATOM	1609	N	LEU	368	71.051	20.812	17.485	1.00	33.86
ATOM	1610	CA	LEU	368	70.144	20.617	18.608	1.00	32.97
ATOM	1611	CB	LEU	368	69.866	19.123	18.759	1.00	34.22
ATOM	1612	CG	LEU	368	68.458	18.633	19.084	1.00	38.15
ATOM	1613	CD1	LEU	368	67.400	19.449	18.345	1.00	27.75
ATOM	1614	CD2	LEU	368	68.374	17.154	18.733	1.00	31.51
ATOM	1615	C	LEU	368	70.793	21.181	19.875	1.00	35.29
ATOM	1616	O	LEU	368	70.128	21.806	20.703	1.00	36.16
ATOM	1617	N	MET	369	72.106	21.001	19.994	1.00	41.13
ATOM	1618	CA	MET	369	72.857	21.504	21.139	1.00	40.92
ATOM	1619	CB	MET	369	74.283	20.955	21.115	1.00	43.32
ATOM	1620	CG	MET	369	74.383	19.497	21.545	1.00	50.01
ATOM	1621	SD	MET	369	75.997	18.770	21.190	1.00	56.63
ATOM	1622	CE	MET	369	77.032	19.596	22.409	1.00	62.26
ATOM	1623	C	MET	369	72.872	23.032	21.186	1.00	43.46
ATOM	1624	O	MET	369	73.137	23.619	22.233	1.00	47.51
ATOM	1625	N	LYS	370	72.594	23.673	20.053	1.00	41.60
ATOM	1626	CA	LYS	370	72.561	25.131	19.988	1.00	34.48
ATOM	1627	CB	LYS	370	72.689	25.623	18.546	1.00	31.53
ATOM	1628	CG	LYS	370	74.012	25.278	17.896	1.00	30.76
ATOM	1629	CD	LYS	370	75.168	25.774	18.731	1.00	32.16
ATOM	1630	CE	LYS	370	76.488	25.388	18.116	1.00	31.08
ATOM	1631	NZ	LYS	370	77.604	25.822	18.993	1.00	51.52
ATOM	1632	C	LYS	370	71.269	25.652	20.606	1.00	36.35
ATOM	1633	O	LYS	370	71.197	26.806	21.032	1.00	39.02
ATOM	1634	N	VAL	371	70.248	24.804	20.652	1.00	34.33
ATOM	1635	CA	VAL	371	68.975	25.186	21.249	1.00	36.27
ATOM	1636	CB	VAL	371	67.885	24.097	21.046	1.00	36.15
ATOM	1637	CG1	VAL	371	66.600	24.487	21.758	1.00	32.69
ATOM	1638	CG2	VAL	371	67.612	23.892	19.567	1.00	33.75
ATOM	1639	C	VAL	371	69.196	25.423	22.745	1.00	41.55
ATOM	1640	O	VAL	371	68.638	26.367	23.316	1.00	40.82
ATOM	1641	N	THR	372	70.018	24.581	23.378	1.00	40.42
ATOM	1642	CA	THR	372	70.300	24.733	24.804	1.00	41.69
ATOM	1643	CB	THR	372	71.037	23.499	25.397	1.00	42.36
ATOM	1644	OG1	THR	372	72.125	23.133	24.548	1.00	53.57
ATOM	1645	CG2	THR	372	70.090	22.313	25.523	1.00	43.54
ATOM	1646	C	THR	372	71.090	26.021	25.048	1.00	38.75
ATOM	1647	O	THR	372	70.858	26.714	26.042		



ATOM	1650	CB	ASP	373	73.741	27.732	23.047	1.00	31.26
ATOM	1651	CG	ASP	373	74.865	26.707	23.085	1.00	35.85
ATOM	1652	OD1	ASP	373	75.523	26.508	22.042	1.00	36.73
ATOM	1653	OD2	ASP	373	75.102	26.103	24.153	1.00	39.92
ATOM	1654	C	ASP	373	71.797	28.769	24.230	1.00	31.30
ATOM	1655	O	ASP	373	71.926	29.689	25.039	1.00	35.37
ATOM	1656	N	LEU	374	70.804	28.711	23.348	1.00	27.72
ATOM	1657	CA	LEU	374	69.783	29.751	23.257	1.00	28.18
ATOM	1658	CB	LEU	374	68.881	29.521	22.042	1.00	28.41
ATOM	1659	CG	LEU	374	69.391	30.055	20.703	1.00	29.87
ATOM	1660	CD1	LEU	374	68.533	29.520	19.563	1.00	25.44
ATOM	1661	CD2	LEU	374	69.385	31.581	20.728	1.00	23.74
ATOM	1662	C	LEU	374	68.946	29.786	24.527	1.00	28.61
ATOM	1663	O	LEU	374	68.516	30.859	24.968	1.00	29.51
ATOM	1664	N	ARG	375	68.690	28.615	25.105	1.00	32.32
ATOM	1665	CA	ARG	375	67.925	28.532	26.345	1.00	33.19
ATOM	1666	CB	ARG	375	67.758	27.074	26.776	1.00	41.70
ATOM	1667	CG	ARG	375	66.360	26.524	26.609	1.00	51.03
ATOM	1668	CD	ARG	375	65.979	26.416	25.153	1.00	60.16
ATOM	1669	NE	ARG	375	64.648	25.840	24.987	1.00	74.28
ATOM	1670	CZ	ARG	375	64.324	24.587	25.296	1.00	79.34
ATOM	1671	NH1	ARG	375	65.233	23.756	25.796	1.00	80.84
ATOM	1672	NH2	ARG	375	63.084	24.157	25.092	1.00	77.44
ATOM	1673	C	ARG	375	68.692	29.296	27.423	1.00	32.02
ATOM	1674	O	ARG	375	68.132	30.150	28.108	1.00	30.42
ATOM	1675	N	MET	376	69.993	29.020	27.521	1.00	32.30
ATOM	1676	CA	MET	376	70.860	29.668	28.499	1.00	36.82
ATOM	1677	CB	MET	376	72.278	29.097	28.433	1.00	45.36
ATOM	1678	CG	MET	376	72.375	27.645	28.866	1.00	66.71
ATOM	1679	SD	MET	376	74.078	27.057	28.966	1.00	89.64
ATOM	1680	CE	MET	376	74.256	26.229	27.400	1.00	85.51
ATOM	1681	C	MET	376	70.880	31.182	28.310	1.00	37.49
ATOM	1682	O	MET	376	70.780	31.928	29.281	1.00	39.99
ATOM	1683	N	ILE	377	71.008	31.630	27.060	1.00	33.14
ATOM	1684	CA	ILE	377	71.009	33.057	26.740	1.00	25.98
ATOM	1685	CB	ILE	377	71.181	33.291	25.211	1.00	22.79
ATOM	1686	CG2	ILE	377	70.838	34.727	24.834	1.00	25.29
ATOM	1687	CG1	ILE	377	72.606	32.947	24.785	1.00	21.42
ATOM	1688	CD1	ILE	377	72.816	32.971	23.282	1.00	19.37
ATOM	1689	C	ILE	377	69.690	33.664	27.228	1.00	27.11
ATOM	1690	O	ILE	377	69.676	34.727	27.856	1.00	28.09
ATOM	1691	N	GLY	378	68.584	32.969	26.975	1.00	29.34
ATOM	1692	CA	GLY	378	67.292	33.457	27.418	1.00	30.41
ATOM	1693	C	GLY	378	67.233	33.532	28.934	1.00	36.85
ATOM	1694	O	GLY	378	66.672	34.481	29.489	1.00	36.44

ATOM	1697	CB	ALA	379	68.415	31.133	31.528	1.00	35.63
ATOM	1698	C	ALA	379	68.712	33.613	31.642	1.00	34.14
ATOM	1699	O	ALA	379	68.259	34.343	32.523	1.00	35.15
ATOM	1700	N	CYA	380	69.941	33.747	31.144	1.00	36.66
ATOM	1701	CA	CYA	380	70.860	34.795	31.587	1.00	37.27
ATOM	1702	CB	CYA	380	72.172	34.728	30.810	1.00	36.85
ATOM	1703	SG	CYA	380	73.201	33.338	31.250	1.00	52.80
ATOM	1704	AS	CYA	380	74.942	33.593	29.823	1.00	65.79
ATOM	1705	C	CYA	380	70.230	36.165	31.398	1.00	38.70
ATOM	1706	O	CYA	380	70.337	37.033	32.270	1.00	45.73
ATOM	1707	N	HIS	381	69.555	36.354	30.265	1.00	37.32
ATOM	1708	CA	HIS	381	68.906	37.623	29.994	1.00	32.11
ATOM	1709	CB	HIS	381	68.377	37.687	28.565	1.00	25.76
ATOM	1710	CG	HIS	381	67.596	38.932	28.285	1.00	20.30
ATOM	1711	CD2	HIS	381	67.998	40.200	28.044	1.00	16.31
ATOM	1712	ND1	HIS	381	66.218	38.971	28.336	1.00	22.06
ATOM	1713	CE1	HIS	381	65.807	40.210	28.146	1.00	21.20
ATOM	1714	NE2	HIS	381	66.869	40.976	27.968	1.00	22.58
ATOM	1715	C	HIS	381	67.773	37.893	30.980	1.00	32.68
ATOM	1716	O	HIS	381	67.602	39.024	31.431	1.00	33.38
ATOM	1717	N	ALA	382	66.982	36.873	31.296	1.00	31.27
ATOM	1718	CA	ALA	382	65.884	37.045	32.243	1.00	29.39
ATOM	1719	CB	ALA	382	65.121	35.742	32.409	1.00	25.18
ATOM	1720	C	ALA	382	66.420	37.531	33.596	1.00	34.32
ATOM	1721	O	ALA	382	65.902	38.501	34.160	1.00	37.79
ATOM	1722	N	SER	383	67.483	36.893	34.085	1.00	36.88
ATOM	1723	CA	SER	383	68.100	37.268	35.361	1.00	39.74
ATOM	1724	CB	SER	383	69.233	36.297	35.719	1.00	42.58
ATOM	1725	OG	SER	383	68.734	35.010	36.049	1.00	61.85
ATOM	1726	C	SER	383	68.638	38.697	35.311	1.00	36.49
ATOM	1727	O	SER	383	68.443	39.480	36.243	1.00	43.81
ATOM	1728	N	ARG	384	69.305	39.036	34.213	1.00	33.66
ATOM	1729	CA	ARG	384	69.866	40.367	34.043	1.00	35.39
ATOM	1730	CB	ARG	384	70.800	40.404	32.835	1.00	29.29
ATOM	1731	CG	ARG	384	71.590	41.679	32.731	1.00	29.20
ATOM	1732	CD	ARG	384	72.881	41.435	31.995	1.00	37.73
ATOM	1733	NE	ARG	384	73.657	42.663	31.850	1.00	48.97
ATOM	1734	CZ	ARG	384	74.346	43.245	32.826	1.00	45.41
ATOM	1735	NH1	ARG	384	74.371	42.715	34.038	1.00	44.51
ATOM	1736	NH2	ARG	384	75.008	44.368	32.584	1.00	41.43
ATOM	1737	C	ARG	384	68.777	41.431	33.916	1.00	39.45
ATOM	1738	O	ARG	384	68.913	42.537	34.444	1.00	44.47
ATOM	1739	N	PHE	385	67.673	41.077	33.270	1.00	36.42
ATOM	1740	CA	PHE	385	66.568	42.007	33.099	1.00	34.68
ATOM	1741	CB	PHE	385	65.444	41.393	32.262	1.00	30.21
ATOM	1								

ATOM	1744	CD2 PHE	385	63.130	42.161	32.873	1.00	28.04
ATOM	1745	CE1 PHE	385	63.203	44.169	30.966	1.00	33.50
ATOM	1746	CE2 PHE	385	62.040	43.012	32.718	1.00	31.35
ATOM	1747	CZ PHE	385	62.077	44.017	31.763	1.00	32.08
ATOM	1748	C PHE	385	66.040	42.412	34.468	1.00	35.76
ATOM	1749	O- PHE	385	65.761	43.590	34.693	1.00	40.58
ATOM	1750	N LEU	386	65.906	41.441	35.373	1.00	37.55
ATOM	1751	CA LEU	386	65.429	41.706	36.735	1.00	41.01
ATOM	1752	CB LEU	386	65.394	40.413	37.563	1.00	42.30
ATOM	1753	CG LEU	386	64.240	39.434	37.317	1.00	43.34
ATOM	1754	CD1 LEU	386	64.559	38.066	37.912	1.00	43.50
ATOM	1755	CD2 LEU	386	62.946	39.992	37.899	1.00	44.01
ATOM	1756	C LEU	386	66.342	42.735	37.405	1.00	40.08
ATOM	1757	O LEU	386	65.875	43.632	38.112	1.00	42.08
ATOM	1758	N HIS	387	67.643	42.613	37.153	1.00	34.86
ATOM	1759	CA HIS	387	68.631	43.537	37.700	1.00	39.09
ATOM	1760	CB HIS	387	70.046	43.034	37.421	1.00	39.99
ATOM	1761	CG HIS	387	70.402	41.791	38.172	1.00	56.37
ATOM	1762	CD2 HIS	387	71.384	40.881	37.974	1.00	60.11
ATOM	1763	ND1 HIS	387	69.711	41.370	39.290	1.00	60.40
ATOM	1764	CE1 HIS	387	70.252	40.255	39.746	1.00	61.89
ATOM	1765	NE2 HIS	387	71.269	39.937	38.966	1.00	63.96
ATOM	1766	C HIS	387	68.446	44.928	37.101	1.00	41.00
ATOM	1767	O HIS	387	68.492	45.927	37.817	1.00	46.99
ATOM	1768	N MET	388	68.213	44.982	35.792	1.00	39.15
ATOM	1769	CA MET	388	68.011	46.243	35.088	1.00	35.32
ATOM	1770	CB MET	388	67.676	45.992	33.612	1.00	35.12
ATOM	1771	CG MET	388	68.810	45.442	32.753	1.00	37.24
ATOM	1772	SD MET	388	68.259	45.150	31.051	1.00	41.75
ATOM	1773	CE MET	388	69.274	43.748	30.573	1.00	35.23
ATOM	1774	C MET	388	66.880	47.048	35.733	1.00	36.52
ATOM	1775	O MET	388	66.994	48.265	35.888	1.00	43.39
ATOM	1776	N LYS	389	65.792	46.371	36.103	1.00	38.05
ATOM	1777	CA LYS	389	64.637	47.025	36.729	1.00	42.88
ATOM	1778	CB LYS	389	63.481	46.035	36.866	1.00	47.83
ATOM	1779	CG LYS	389	62.835	45.627	35.560	1.00	52.36
ATOM	1780	CD LYS	389	62.040	44.340	35.731	1.00	61.84
ATOM	1781	CE LYS	389	60.978	44.451	36.814	1.00	69.04
ATOM	1782	NZ LYS	389	60.254	43.162	36.987	1.00	70.00
ATOM	1783	C LYS	389	64.983	47.587	38.107	1.00	43.99
ATOM	1784	O LYS	389	64.455	48.621	38.525	1.00	44.22
ATOM	1785	N VAL	390	65.851	46.878	38.816	1.00	45.50
ATOM	1786	CA VAL	390	66.290	47.286	40.142	1.00	47.76
ATOM	1787	CB VAL	390	67.152	46.186	40.804	1.00	46.30
ATOM	1788	CG1 VAL	390	67.796	46.706	42.079	1.00	49.20
ATOM	1789	CG2 VAL	390	66.305	44.962	41.097	1.00	42.69
ATOM	1790	C VAL	390	67.109	48.571	40.070	1.00	47.25

ATOM	1791	O	VAL	390	66.811	49.540	40.760	1.00	48.67
ATOM	1792	N	GLU	391	68.115	48.580	39.199	1.00	44.11
ATOM	1793	CA	GLU	391	69.009	49.721	39.047	1.00	45.79
ATOM	1794	CB	GLU	391	70.266	49.311	38.273	1.00	45.78
ATOM	1795	CG	GLU	391	70.998	48.091	38.830	1.00	57.29
ATOM	1796	CD	GLU	391	71.479	48.268	40.261	1.00	61.20
ATOM	1797	OE1	GLU	391	71.845	49.400	40.646	1.00	57.29
ATOM	1798	OE2	GLU	391	71.496	47.263	41.001	1.00	63.69
ATOM	1799	C	GLU	391	68.410	50.959	38.391	1.00	49.16
ATOM	1800	O	GLU	391	68.463	52.055	38.956	1.00	58.82
ATOM	1801	N	CYA	392	67.802	50.782	37.224	1.00	49.75
ATOM	1802	CA	CYA	392	67.255	51.908	36.475	1.00	45.56
ATOM	1803	CB	CYA	392	67.667	51.768	35.016	1.00	44.82
ATOM	1804	SG	CYA	392	69.443	51.771	34.913	1.00	50.78
ATOM	1805	AS	CYA	392	69.929	50.778	33.022	1.00	53.29
ATOM	1806	C	CYA	392	65.771	52.200	36.601	1.00	44.35
ATOM	1807	O	CYA	392	64.988	51.324	36.962	1.00	44.10
ATOM	1808	N	PRO	393	65.378	53.469	36.365	1.00	45.52
ATOM	1809	CD	PRO	393	66.275	54.603	36.075	1.00	37.38
ATOM	1810	CA	PRO	393	63.982	53.916	36.444	1.00	45.41
ATOM	1811	CB	PRO	393	64.105	55.438	36.376	1.00	43.33
ATOM	1812	CG	PRO	393	65.329	55.644	35.542	1.00	39.89
ATOM	1813	C	PRO	393	63.108	53.376	35.318	1.00	44.89
ATOM	1814	O	PRO	393	63.556	53.239	34.175	1.00	45.60
ATOM	1815	N	THR	394	61.843	53.135	35.647	1.00	47.52
ATOM	1816	CA	THR	394	60.853	52.603	34.713	1.00	53.06
ATOM	1817	CB	THR	394	59.459	52.583	35.371	1.00	61.06
ATOM	1818	OG1	THR	394	59.609	52.470	36.794	1.00	72.44
ATOM	1819	CG2	THR	394	58.640	51.401	34.860	1.00	61.05
ATOM	1820	C	THR	394	60.767	53.373	33.392	1.00	49.98
ATOM	1821	O	THR	394	60.507	52.786	32.339	1.00	51.06
ATOM	1822	N	GLU	395	61.024	54.676	33.452	1.00	48.55
ATOM	1823	CA	GLU	395	60.970	55.548	32.282	1.00	44.21
ATOM	1824	CB	GLU	395	61.258	56.987	32.697	1.00	41.66
ATOM	1825	C	GLU	395	61.899	55.134	31.134	1.00	43.46
ATOM	1826	O	GLU	395	61.684	55.527	29.988	1.00	44.17
ATOM	1827	N	LEU	396	62.934	54.359	31.449	1.00	41.05
ATOM	1828	CA	LEU	396	63.898	53.899	30.448	1.00	39.55
ATOM	1829	CB	LEU	396	65.270	53.708	31.106	1.00	35.03
ATOM	1830	CG	LEU	396	66.296	54.834	30.945	1.00	40.06
ATOM	1831	CD1	LEU	396	65.638	56.200	31.055	1.00	39.06
ATOM	1832	CD2	LEU	396	67.398	54.669	31.978	1.00	32.78
ATOM	1833	C	LEU	396	63.468	52.602	29.757	1.00	38.50
ATOM	1834	O	LEU	396	64.106	52.150	28.804	1.00	34.72
ATOM	1835	N	PHE	397	62.364	52.028	30.225	1.00	3



ATOM	1838	CG	PHE	397	62.842	49.421	31.607	1.00	36.95
ATOM	1839	CD1	PHE	397	63.331	50.280	32.587	1.00	34.61
ATOM	1840	CD2	PHE	397	63.523	48.234	31.362	1.00	37.14
ATOM	1841	CE1	PHE	397	64.481	49.964	33.310	1.00	31.57
ATOM	1842	CE2	PHE	397	64.675	47.908	32.082	1.00	37.85
ATOM	1843	CZ	PHE	397	65.153	48.776	33.056	1.00	33.08
ATOM	1844	C	PHE	397	60.584	50.921	28.858	1.00	35.65
ATOM	1845	O	PHE	397	59.519	51.249	29.399	1.00	35.75
ATOM	1846	N	PRO	398	60.672	50.685	27.536	1.00	35.78
ATOM	1847	CD	PRO	398	61.891	50.367	26.767	1.00	32.81
ATOM	1848	CA	PRO	398	59.503	50.786	26.658	1.00	33.94
ATOM	1849	CB	PRO	398	60.041	50.297	25.315	1.00	33.91
ATOM	1850	CG	PRO	398	61.488	50.707	25.356	1.00	33.09
ATOM	1851	C	PRO	398	58.434	49.840	27.210	1.00	34.98
ATOM	1852	O	PRO	398	58.753	48.729	27.654	1.00	35.76
ATOM	1853	N	PRO	399	57.163	50.267	27.219	1.00	37.67
ATOM	1854	CD	PRO	399	56.661	51.578	26.776	1.00	38.02
ATOM	1855	CA	PRO	399	56.070	49.433	27.733	1.00	36.86
ATOM	1856	CB	PRO	399	54.803	50.183	27.291	1.00	34.14
ATOM	1857	CG	PRO	399	55.282	51.240	26.310	1.00	37.00
ATOM	1858	C	PRO	399	56.085	47.970	27.273	1.00	37.06
ATOM	1859	O	PRO	399	55.967	47.063	28.099	1.00	37.07
ATOM	1860	N	LEU	400	56.299	47.738	25.980	1.00	35.13
ATOM	1861	CA	LEU	400	56.327	46.374	25.445	1.00	35.86
ATOM	1862	CB	LEU	400	56.314	46.385	23.914	1.00	31.49
ATOM	1863	CG	LEU	400	56.181	45.017	23.227	1.00	30.73
ATOM	1864	CD1	LEU	400	54.901	44.330	23.674	1.00	21.35
ATOM	1865	CD2	LEU	400	56.197	45.183	21.720	1.00	25.42
ATOM	1866	C	LEU	400	57.542	45.597	25.958	1.00	36.51
ATOM	1867	O	LEU	400	57.458	44.392	26.219	1.00	37.47
ATOM	1868	N	PHE	401	58.671	46.290	26.095	1.00	32.26
ATOM	1869	CA	PHE	401	59.899	45.682	26.596	1.00	35.15
ATOM	1870	CB	PHE	401	61.014	46.739	26.648	1.00	35.99
ATOM	1871	CG	PHE	401	62.346	46.213	27.117	1.00	39.41
ATOM	1872	CD1	PHE	401	62.845	45.003	26.639	1.00	35.94
ATOM	1873	CD2	PHE	401	63.119	46.944	28.019	1.00	40.55
ATOM	1874	CE1	PHE	401	64.088	44.531	27.055	1.00	30.16
ATOM	1875	CE2	PHE	401	64.367	46.478	28.439	1.00	35.53
ATOM	1876	CZ	PHE	401	64.849	45.271	27.952	1.00	36.39
ATOM	1877	C	PHE	401	59.607	45.129	27.996	1.00	36.42
ATOM	1878	O	PHE	401	59.957	43.995	28.317	1.00	36.71
ATOM	1879	N	LEU	402	58.920	45.925	28.805	1.00	36.59
ATOM	1880	CA	LEU	402	58.561	45.528	30.158	1.00	37.68
ATOM	1881	CB	LEU	402	57.986	46.720	30.917	1.00	40.71
ATOM	1882	CG	LEU	402	58.963	47.751	31.463	1.00	43



ATOM	1885	C	LEU	402	57.521	44.420	30.164	1.00	38.02
ATOM	1886	O	LEU	402	57.582	43.507	30.984	1.00	37.39
ATOM	1887	N	GLU	403	56.558	44.522	29.251	1.00	39.74
ATOM	1888	CA	GLU	403	55.469	43.559	29.166	1.00	42.79
ATOM	1889	CB	GLU	403	54.445	44.022	28.129	1.00	46.21
ATOM	1890	CG	GLU	403	53.092	43.330	28.232	1.00	56.88
ATOM	1891	CD	GLU	403	52.090	43.833	27.202	1.00	65.21
ATOM	1892	OE1	GLU	403	52.230	44.983	26.728	1.00	70.60
ATOM	1893	OE2	GLU	403	51.154	43.073	26.870	1.00	70.53
ATOM	1894	C	GLU	403	55.890	42.121	28.886	1.00	40.14
ATOM	1895	O	GLU	403	55.368	41.200	29.506	1.00	40.57
ATOM	1896	N	VAL	404	56.835	41.932	27.966	1.00	39.43
ATOM	1897	CA	VAL	404	57.292	40.586	27.610	1.00	40.96
ATOM	1898	CB	VAL	404	57.851	40.516	26.159	1.00	35.50
ATOM	1899	CG1	VAL	404	56.807	40.995	25.177	1.00	43.46
ATOM	1900	CG2	VAL	404	59.132	41.321	26.030	1.00	25.74
ATOM	1901	C	VAL	404	58.317	39.946	28.536	1.00	41.94
ATOM	1902	O	VAL	404	58.468	38.722	28.533	1.00	43.82
ATOM	1903	N	PHE	405	59.026	40.759	29.310	1.00	39.84
ATOM	1904	CA	PHE	405	60.051	40.223	30.189	1.00	42.73
ATOM	1905	CB	PHE	405	61.401	40.897	29.913	1.00	36.85
ATOM	1906	CG	PHE	405	61.963	40.596	28.551	1.00	33.23
ATOM	1907	CD1	PHE	405	62.283	41.625	27.672	1.00	33.90
ATOM	1908	CD2	PHE	405	62.157	39.281	28.138	1.00	31.62
ATOM	1909	CE1	PHE	405	62.786	41.351	26.399	1.00	39.16
ATOM	1910	CE2	PHE	405	62.657	38.997	26.872	1.00	33.33
ATOM	1911	CZ	PHE	405	62.972	40.033	25.999	1.00	31.99
ATOM	1912	C	PHE	405	59.723	40.273	31.676	1.00	43.97
ATOM	1913	O	PHE	405	60.636	39.943	32.460	1.00	46.56
ATOM	1	O1	HOH	501	67.928	36.755	11.188	1.00	33.04
ATOM	2	O1	HOH	502	69.618	40.719	13.009	1.00	23.00
ATOM	3	O1	HOH	503	64.885	40.168	12.340	1.00	23.00
ATOM	4	O1	HOH	504	63.079	40.108	15.841	1.00	23.00
ATOM	5	O1	HOH	505	63.404	46.536	15.354	1.00	36.41
ATOM	6	O1	HOH	506	61.299	15.617	-0.595	1.00	23.00
ATOM	7	O1	HOH	507	67.359	15.375	0.551	1.00	23.00
ATOM	8	O1	HOH	508	67.230	12.002	-0.634	1.00	23.00
ATOM	9	O1	HOH	509	66.906	12.467	3.855	1.00	23.00
ATOM	10	O1	HOH	510	61.785	9.946	3.983	1.00	23.00
ATOM	11	O1	HOH	511	57.670	11.385	9.909	1.00	23.00
ATOM	12	O1	HOH	512	55.791	11.570	10.291	1.00	23.00
ATOM	13	O1	HOH	513	54.637	14.058	9.201	1.00	23.00
ATOM	14	O1	HOH	514	55.882	16.054	12.204	1.00	26.53
ATOM	15	O1	HOH	515	53.685	15.842	18.209	1.00	23.00
ATOM	16	O1	HOH	516	49.559	24.773	19.020	1.00	23.00
ATOM	17	O1	HO						

ATOM	19	O1	HOH	519	50.338	23.299	7.662	1.00	41.19
ATOM	20	O1	HOH	520	50.830	20.272	8.323	1.00	28.46
ATOM	21	O1	HOH	521	48.630	20.291	6.429	1.00	23.00
ATOM	22	O1	HOH	522	49.233	17.389	2.867	1.00	23.00
ATOM	23	O1	HOH	523	52.076	22.770	1.260	1.00	23.00
ATOM	24	O1	HOH	524	51.671	23.621	-1.020	1.00	23.00
ATOM	25	O1	HOH	525	58.294	31.509	2.147	1.00	31.83
ATOM	26	O1	HOH	526	57.497	36.071	2.268	1.00	23.00
ATOM	27	O1	HOH	527	65.373	36.025	6.809	1.00	23.00
ATOM	28	O1	HOH	528	67.871	36.399	6.419	1.00	66.52
ATOM	29	O1	HOH	529	67.189	33.811	9.409	1.00	23.00
ATOM	30	O1	HOH	530	62.458	48.056	13.590	1.00	23.00
ATOM	31	O1	HOH	531	63.943	46.824	10.638	1.00	39.26
ATOM	32	O1	HOH	532	57.465	45.867	13.186	1.00	23.00
ATOM	33	O1	HOH	533	55.223	40.774	10.959	1.00	23.00
ATOM	34	O1	HOH	534	53.737	44.032	19.560	1.00	23.00
ATOM	35	O1	HOH	535	55.982	49.757	24.168	1.00	23.00
ATOM	36	O1	HOH	536	58.575	52.330	31.881	1.00	23.00
ATOM	37	O1	HOH	537	62.563	49.327	37.804	1.00	23.00
ATOM	38	O1	HOH	538	61.736	40.280	35.059	1.00	60.53
ATOM	39	O1	HOH	539	63.271	38.155	34.156	1.00	52.21
ATOM	40	O1	HOH	540	61.872	35.187	29.990	1.00	23.00
ATOM	41	O1	HOH	541	63.701	36.808	28.720	1.00	23.00
ATOM	42	O1	HOH	542	62.255	35.864	26.425	1.00	26.69
ATOM	43	O1	HOH	543	63.567	33.453	25.308	1.00	44.90
ATOM	44	O1	HOH	544	65.456	30.135	27.713	1.00	23.00
ATOM	45	O1	HOH	545	61.997	26.566	24.157	1.00	23.00
ATOM	46	O1	HOH	546	61.422	22.231	24.358	1.00	23.00
ATOM	47	O1	HOH	547	59.636	21.462	25.378	1.00	23.00
ATOM	48	O1	HOH	548	64.860	21.210	22.578	1.00	23.00
ATOM	49	O1	HOH	549	63.316	14.964	15.508	1.00	52.55
ATOM	50	O1	HOH	550	62.770	10.707	15.710	1.00	48.78
ATOM	51	O1	HOH	551	61.579	9.665	12.081	1.00	23.00
ATOM	52	O1	HOH	552	65.916	11.929	11.639	1.00	23.00
ATOM	53	O1	HOH	553	68.086	12.882	11.226	1.00	23.00
ATOM	54	O1	HOH	554	69.504	11.968	14.083	1.00	23.00
ATOM	55	O1	HOH	555	72.311	15.121	10.552	1.00	23.00
ATOM	56	O1	HOH	556	74.716	15.172	10.253	1.00	23.00
ATOM	57	O1	HOH	557	73.109	17.916	7.451	1.00	23.00
ATOM	58	O1	HOH	558	71.316	15.446	7.652	1.00	23.00
ATOM	59	O1	HOH	559	74.717	14.555	5.957	1.00	23.00
ATOM	60	O1	HOH	560	73.523	22.311	2.467	1.00	23.00
ATOM	61	O1	HOH	561	76.491	23.094	5.700	1.00	51.34
ATOM	62	O1	HOH	562	73.961	29.841	10.035	1.00	33.87
ATOM	63	O1	HOH	563	76.164	33.031	11.370	1.00	23.00
ATOM	64	O1	HOH	564	77.193	34.039	9.712	1.00	37.14
ATOM	65	O1	HOH	565	76.525	41.395	10.460	1.00	23.00

ATOM	66	O1	HOH	566	79.358	49.535	15.048	1.00	53.78
ATOM	67	O1	HOH	567	78.046	53.530	9.188	1.00	23.00
ATOM	68	O1	HOH	568	68.058	52.158	15.548	1.00	23.00
ATOM	69	O1	HOH	569	68.598	53.164	18.083	1.00	45.72
ATOM	70	O1	HOH	570	73.482	58.914	21.552	1.00	58.99
ATOM	71	O1	HOH	571	65.648	53.551	26.240	1.00	23.00
ATOM	72	O1	HOH	572	75.776	46.207	30.367	1.00	33.32
ATOM	73	O1	HOH	573	78.686	46.470	31.087	1.00	23.00
ATOM	74	O1	HOH	574	77.580	41.209	31.884	1.00	23.00
ATOM	75	O1	HOH	575	76.879	31.531	24.067	1.00	23.00
ATOM	76	O1	HOH	576	77.927	29.163	20.647	1.00	23.00
ATOM	77	O1	HOH	577	80.180	24.963	17.233	1.00	53.36
ATOM	78	O1	HOH	578	80.631	25.802	15.508	1.00	23.00
ATOM	79	O1	HOH	579	82.104	22.566	14.156	1.00	23.00
ATOM	80	O1	HOH	580	76.954	22.077	18.425	1.00	46.50
ATOM	81	O1	HOH	581	86.619	37.903	16.945	1.00	47.66
ATOM	82	O1	HOH	582	83.586	42.305	18.576	1.00	23.00
ATOM	83	O1	HOH	583	83.481	45.262	19.526	1.00	23.00
ATOM	84	O1	HOH	584	66.787	32.864	33.796	1.00	23.00
ATOM	85	O1	HOH	585	59.447	33.572	30.734	1.00	23.00
ATOM	86	O1	HOH	586	57.013	32.278	31.125	1.00	23.00
ATOM	87	O1	HOH	587	58.084	29.428	24.648	1.00	24.06
ATOM	88	O1	HOH	588	52.774	25.054	32.650	1.00	57.81
ATOM	89	O1	HOH	589	53.800	24.465	34.834	1.00	23.00
ATOM	90	O1	HOH	590	47.195	30.205	30.414	1.00	23.00
ATOM	91	O1	HOH	591	48.978	35.051	30.228	1.00	23.00
ATOM	92	O1	HOH	592	49.280	39.962	31.041	1.00	23.00
ATOM	93	O1	HOH	593	42.329	32.230	20.993	1.00	23.00
ATOM	94	O1	HOH	594	44.199	32.910	19.088	1.00	23.00
ATOM	95	O1	HOH	595	41.542	27.336	19.178	1.00	23.00
ATOM	96	O1	HOH	596	48.971	31.296	14.022	1.00	23.00
ATOM	97	O1	HOH	597	50.180	31.092	7.307	1.00	23.00
ATOM	98	O1	HOH	598	64.465	28.209	3.208	1.00	45.35
ATOM	99	O1	HOH	599	67.740	26.910	1.986	1.00	23.00
ATOM	100	O1	HOH	600	67.958	31.203	3.532	1.00	23.00
ATOM	101	O1	HOH	601	68.885	22.721	0.234	1.00	39.53
ATOM	102	O1	HOH	602	46.735	20.335	25.877	1.00	44.92
ATOM	103	O1	HOH	603	47.359	19.644	28.494	1.00	41.57
ATOM	2300	C	ACY	701	52.555	39.909	24.622	1.00	48.75
ATOM	2301	O	ACY	701	52.351	40.361	25.771	1.00	48.92
ATOM	2302	OXT	ACY	701	53.503	39.156	24.279	1.00	50.69
ATOM	2303	CH3	ACY	701	51.543	40.314	23.527	1.00	41.32
ATOM	2304	C1	IBR	1	67.309	42.207	18.510	1.00	32.20
ATOM	2305	C2	IBR	1	68.795	43.194	23.237	1.00	29.59
ATOM	2306	C3	IBR	1	67.192	43.467	19.068	1.00	25.49
ATOM	2307	C4	IBR	1	69.09				

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ATOM 2309 C6 IBR 1 68.489 44.345 25.356 1.00 30.87
ATOM 2310 C7 IBR 1 68.673 42.828 20.790 1.00 30.76
ATOM 2311 C8 IBR 1 67.681 43.327 25.704 1.00 29.18
ATOM 2312 C9 IBR 1 68.811 41.580 20.269 1.00 32.19
ATOM 2313 C10 IBR 1 67.383 42.244 24.921 1.00 26.78
ATOM 2314 C11 IBR 1 68.122 41.241 19.099 1.00 25.50
ATOM 2315 C12 IBR 1 67.979 42.171 23.609 1.00 24.47
ATOM 2316 C13 IBR 1 66.529 41.932 17.285 1.00 17.69
ATOM 2317 C14 IBR 1 68.730 45.450 26.287 1.00 30.43
ATOM 2318 C15 IBR 1 67.011 40.785 16.271 1.00 21.37
ATOM 2319 C16 IBR 1 67.939 46.867 25.912 1.00 23.75
ATOM 2320 C17 IBR 1 65.946 40.598 15.151 1.00 23.91
ATOM 2321 C18 IBR 1 70.126 46.087 26.069 1.00 26.02
ATOM 2322 BR1 IBR 1 67.708 45.504 20.878 1.00 34.64
ATOM 2323 BR2 IBR 1 69.927 40.301 21.039 1.00 32.01
ATOM 2324 N1 IBR 1 68.284 40.938 15.821 1.00 18.75
ATOM 2325 O1 IBR 1 67.068 43.397 26.981 1.00 26.31
ATOM 2326 O2 IBR 1 69.393 43.153 21.933 1.00 30.15
ATOM 2327 O3 IBR 1 66.368 40.592 14.004 1.00 23.29
ATOM 2328 O4 IBR 1 64.786 40.511 15.515 1.00 23.47
END
END

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# APPENDIX 6

## TR\_T3.PDB

REMARK rTR\_t3 full length numbering

REMARK

REMARK Rfactor 0.221 Rfree 0.240

REMARK Resolution 5. 2.0 all reflections

REMARK conformation of MET 388 confirmed by SA\_omit map

REMARK

REMARK Three cacodylate-modified cysteines (CYA)

REMARK Cya334, Cya380, Cya392

REMARK cacodylate modeled as single arsenic atom

REMARK

REMARK side chain of certain residues modeled as ALA due to poor density;

REMARK however, residue name reflects true residue for clarity

REMARK

REMARK clone obtained from Murray et. al.

REMARK deposited sequence confirmed,

REMARK differing from that reported by Thompson et. al.

REMARK in the following codons:

REMARK 281 Thr - Ala

REMARK 285 Lys - Glu

REMARK identical to that reported by Mitsuhashi et. al.

REMARK gb:RNTRAVI X07409

JRNL AUTH M.B. MURRAY, N.D.ZILZ, N.L.MCCREARY,M.J.MACDONALD

JRNL AUTH 2 H.C.TOWLE

JRNL TITL ISOLATION AND CHARACTERIZATION OF RAT CDNA CLONES  
FOR TWO

JRNL TITL 2 DISTINCT THYROID HORMONE RECPTORS

JRNL REF JBC V. 263 25 1988

JRNL AUTH C.C.THOMPSON, C.WEINBERGER, R.LEBO, R.M.EVANS

JRNL TITL IDENTIFICATION OF A NOVEL THYROID HORMONE RECEPTOR  
EXPRESSED

JRNL TITL 2 IN THE MAMMALIAN CENTRAL NERVOUS SYSTEM

JRNL REF SCIENCE V. 237 1987

JRNL AUTH T.MITSUHASHI,G.TENNYSON,V.NIKODEM

JRNL TITL NUCLEOTIDE SEQUENCE OF NOVEL CDNAS GENERATED BY  
ALTERNATIVE

JRNL TITL 2 SPLICING OF A RAT THYROID HORMONE RECEPTOR GENE  
TRANSCRIPT

JRNL REF NUC. ACIDS. RES. V. 16 12 1988

REMARK

ATOM	1	CB	ARG	157	68.406	10.620	7.027	1.00	41.66
ATOM	2	CG	ARG	157	69.926	10.540	6.997	1.00	44.48
ATOM	3	CD	ARG	157	70.552	11.261	8.173	1.00	47.02
ATOM	4	NE	ARG	157	70.112	10.680	9.435	1.00	49.73



ATOM	5	CZ	ARG	157	70.917	10.392	10.450	1.00	51.21
ATOM	6	NH1	ARG	157	72.223	10.629	10.361	1.00	51.79
ATOM	7	NH2	ARG	157	70.405	9.871	11.556	1.00	51.92
ATOM	8	C	ARG	157	66.308	9.993	5.774	1.00	36.48
ATOM	9	O	ARG	157	66.047	10.318	4.622	1.00	38.84
ATOM	10	N	ARG	157	68.479	9.473	4.839	1.00	41.22
ATOM	11	CA	ARG	157	67.734	9.580	6.135	1.00	39.98
ATOM	12	N	PRO	158	65.366	9.953	6.728	1.00	33.85
ATOM	13	CD	PRO	158	65.494	9.553	8.139	1.00	34.72
ATOM	14	CA	PRO	158	63.981	10.336	6.407	1.00	31.89
ATOM	15	CB	PRO	158	63.219	10.015	7.694	1.00	31.87
ATOM	16	CG	PRO	158	64.260	10.158	8.759	1.00	33.55
ATOM	17	C	PRO	158	63.758	11.783	5.947	1.00	29.77
ATOM	18	O	PRO	158	64.221	12.739	6.575	1.00	27.93
ATOM	19	N	GLU	159	63.071	11.918	4.819	1.00	26.20
ATOM	20	CA	GLU	159	62.759	13.217	4.239	1.00	24.07
ATOM	21	CB	GLU	159	62.565	13.080	2.721	1.00	22.90
ATOM	22	CG	GLU	159	63.847	12.933	1.916	1.00	22.04
ATOM	23	CD	GLU	159	64.386	14.260	1.427	1.00	22.07
ATOM	24	OE1	GLU	159	63.577	15.175	1.203	1.00	24.63
ATOM	25	OE2	GLU	159	65.612	14.389	1.240	1.00	23.54
ATOM	26	C	GLU	159	61.463	13.717	4.855	1.00	21.56
ATOM	27	O	GLU	159	60.747	12.958	5.516	1.00	21.03
ATOM	28	N	PRO	160	61.176	15.022	4.713	1.00	19.69
ATOM	29	CD	PRO	160	61.997	16.139	4.207	1.00	16.57
ATOM	30	CA	PRO	160	59.923	15.500	5.292	1.00	18.12
ATOM	31	CB	PRO	160	59.935	16.990	4.955	1.00	15.65
ATOM	32	CG	PRO	160	61.390	17.328	4.905	1.00	14.83
ATOM	33	C	PRO	160	58.741	14.782	4.626	1.00	19.79
ATOM	34	O	PRO	160	58.793	14.431	3.445	1.00	20.20
ATOM	35	N	THR	161	57.713	14.497	5.412	1.00	20.15
ATOM	36	CA	THR	161	56.525	13.846	4.901	1.00	20.73
ATOM	37	CB	THR	161	55.672	13.274	6.060	1.00	20.77
ATOM	38	OG1	THR	161	55.195	14.348	6.881	1.00	21.74
ATOM	39	CG2	THR	161	56.489	12.324	6.917	1.00	19.52
ATOM	40	C	THR	161	55.724	14.954	4.219	1.00	21.64
ATOM	41	O	THR	161	56.010	16.139	4.421	1.00	23.13
ATOM	42	N	PRO	162	54.701	14.596	3.425	1.00	21.21
ATOM	43	CD	PRO	162	54.309	13.235	3.012	1.00	19.57
ATOM	44	CA	PRO	162	53.884	15.602	2.751	1.00	21.01
ATOM	45	CB	PRO	162	52.722	14.776	2.223	1.00	19.74
ATOM	46	CG	PRO	162	53.387	13.490	1.861	1.00	20.34
ATOM	47	C	PRO	162	53.391	16.643	3.753	1.00	22.52
ATOM	48	O	PRO	162	53.508	17.851	3.526	1.00	21.68
ATOM	49	N	GLU	163	52.880	16.151	4.878	1.00	23.01
ATOM	50	CA	GLU	163	52.349	16.996	5.941	1.00	25.97
ATOM	51	CB	GLU	163	51.672	16.148</			

ATOM	52	CG	GLU	163	50.476	15.312	6.543	1.00	37.07
ATOM	53	CD	GLU	163	50.865	14.159	5.614	1.00	41.36
ATOM	54	OE1	GLU	163	51.937	13.544	5.828	1.00	40.11
ATOM	55	OE2	GLU	163	50.094	13.874	4.660	1.00	46.16
ATOM	56	C	GLU	163	53.415	17.879	6.581	1.00	24.92
ATOM	57	O	GLU	163	53.110	18.971	7.061	1.00	25.82
ATOM	58	N	GLU	164	54.661	17.412	6.600	1.00	22.87
ATOM	59	CA	GLU	164	55.724	18.209	7.187	1.00	21.46
ATOM	60	CB	GLU	164	56.880	17.340	7.664	1.00	21.23
ATOM	61	CG	GLU	164	56.509	16.508	8.886	1.00	20.30
ATOM	62	CD	GLU	164	57.557	15.483	9.243	1.00	20.07
ATOM	63	OE1	GLU	164	58.409	15.186	8.385	1.00	19.80
ATOM	64	OE2	GLU	164	57.532	14.977	10.385	1.00	21.00
ATOM	65	C	GLU	164	56.195	19.289	6.235	1.00	22.45
ATOM	66	O	GLU	164	56.607	20.354	6.684	1.00	23.36
ATOM	67	N	TRP	165	56.140	19.024	4.928	1.00	21.06
ATOM	68	CA	TRP	165	56.518	20.031	3.936	1.00	19.57
ATOM	69	CB	TRP	165	56.486	19.466	2.518	1.00	16.06
ATOM	70	CG	TRP	165	57.775	18.839	2.120	1.00	14.01
ATOM	71	CD2	TRP	165	59.055	19.480	2.037	1.00	13.26
ATOM	72	CE2	TRP	165	59.976	18.515	1.588	1.00	12.91
ATOM	73	CE3	TRP	165	59.507	20.779	2.300	1.00	14.44
ATOM	74	CD1	TRP	165	57.972	17.544	1.738	1.00	12.89
ATOM	75	NE1	TRP	165	59.290	17.343	1.413	1.00	12.80
ATOM	76	CZ2	TRP	165	61.328	18.805	1.388	1.00	15.06
ATOM	77	CZ3	TRP	165	60.850	21.069	2.103	1.00	14.72
ATOM	78	CH2	TRP	165	61.747	20.084	1.649	1.00	16.82
ATOM	79	C	TRP	165	55.553	21.210	4.056	1.00	18.93
ATOM	80	O	TRP	165	55.960	22.359	3.926	1.00	21.12
ATOM	81	N	ASP	166	54.279	20.922	4.307	1.00	19.33
ATOM	82	CA	ASP	166	53.262	21.963	4.483	1.00	20.35
ATOM	83	CB	ASP	166	51.864	21.353	4.672	1.00	20.22
ATOM	84	CG	ASP	166	51.302	20.748	3.386	1.00	23.36
ATOM	85	OD1	ASP	166	51.746	21.153	2.296	1.00	23.42
ATOM	86	OD2	ASP	166	50.414	19.878	3.462	1.00	21.02
ATOM	87	C	ASP	166	53.623	22.785	5.712	1.00	21.02
ATOM	88	O	ASP	166	53.627	24.013	5.654	1.00	22.56
ATOM	89	N	LEU	167	53.926	22.096	6.813	1.00	20.50
ATOM	90	CA	LEU	167	54.312	22.726	8.071	1.00	21.37
ATOM	91	CB	LEU	167	54.661	21.657	9.109	1.00	23.49
ATOM	92	CG	LEU	167	54.223	21.846	10.565	1.00	27.19
ATOM	93	CD1	LEU	167	55.312	21.291	11.453	1.00	27.70
ATOM	94	CD2	LEU	167	53.940	23.314	10.906	1.00	27.71
ATOM	95	C	LEU	167	55.541	23.602	7.839	1.00	20.72
ATOM	96	O	LEU	167	55.601	24.748	8.294	1.00	22.98
ATOM	97	N	ILE	168	56.505	23.051	7.114	1.00	18.54

ATOM	99	CB	ILE	168	58.671	22.771	5.995	1.00	17.54
ATOM	100	CG2	ILE	168	59.695	23.533	5.163	1.00	17.65
ATOM	101	CG1	ILE	168	59.330	21.794	6.972	1.00	20.27
ATOM	102	CD1	ILE	168	60.048	20.631	6.322	1.00	17.96
ATOM	103	C	ILE	168	57.486	25.002	5.979	1.00	21.96
ATOM	104	O	ILE	168	58.045	26.064	6.291	1.00	23.06
ATOM	105	N	HIS	169	56.591	24.925	4.996	1.00	22.04
ATOM	106	CA	HIS	169	56.285	26.092	4.164	1.00	21.21
ATOM	107	CB	HIS	169	55.413	25.702	2.969	1.00	20.12
ATOM	108	CG	HIS	169	56.101	24.799	2.001	1.00	19.18
ATOM	109	CD2	HIS	169	57.398	24.733	1.619	1.00	18.62
ATOM	110	ND1	HIS	169	55.457	23.764	1.357	1.00	17.90
ATOM	111	CE1	HIS	169	56.327	23.096	0.625	1.00	18.43
ATOM	112	NE2	HIS	169	57.513	23.660	0.772	1.00	20.10
ATOM	113	C	HIS	169	55.615	27.198	4.959	1.00	20.61
ATOM	114	O	HIS	169	55.979	28.370	4.836	1.00	20.08
ATOM	115	N	VAL	170	54.632	26.821	5.769	1.00	20.01
ATOM	116	CA	VAL	170	53.922	27.785	6.580	1.00	20.52
ATOM	117	CB	VAL	170	52.816	27.120	7.384	1.00	21.33
ATOM	118	CG1	VAL	170	52.224	28.113	8.366	1.00	22.32
ATOM	119	CG2	VAL	170	51.740	26.608	6.438	1.00	23.27
ATOM	120	C	VAL	170	54.891	28.477	7.521	1.00	20.58
ATOM	121	O	VAL	170	54.926	29.704	7.554	1.00	22.32
ATOM	122	N	ALA	171	55.712	27.696	8.230	1.00	18.83
ATOM	123	CA	ALA	171	56.692	28.234	9.182	1.00	18.34
ATOM	124	CB	ALA	171	57.375	27.102	9.946	1.00	17.05
ATOM	125	C	ALA	171	57.733	29.151	8.533	1.00	17.84
ATOM	126	O	ALA	171	58.084	30.200	9.091	1.00	18.67
ATOM	127	N	THR	172	58.231	28.756	7.367	1.00	17.81
ATOM	128	CA	THR	172	59.215	29.551	6.639	1.00	18.88
ATOM	129	CB	THR	172	59.726	28.794	5.380	1.00	20.47
ATOM	130	OG1	THR	172	60.280	27.531	5.776	1.00	21.38
ATOM	131	CG2	THR	172	60.806	29.599	4.648	1.00	20.22
ATOM	132	C	THR	172	58.655	30.932	6.251	1.00	19.42
ATOM	133	O	THR	172	59.320	31.957	6.435	1.00	17.98
ATOM	134	N	GLU	173	57.425	30.970	5.756	1.00	19.97
ATOM	135	CA	GLU	173	56.811	32.236	5.374	1.00	22.51
ATOM	136	CB	GLU	173	55.520	31.981	4.577	1.00	27.26
ATOM	137	CG	GLU	173	54.823	33.244	4.005	1.00	34.96
ATOM	138	CD	GLU	173	55.690	34.040	3.020	1.00	39.54
ATOM	139	OE1	GLU	173	56.610	33.454	2.395	1.00	41.82
ATOM	140	OE2	GLU	173	55.443	35.259	2.872	1.00	41.06
ATOM	141	C	GLU	173	56.538	33.099	6.622	1.00	21.60
ATOM	142	O	GLU	173	56.726	34.313	6.595	1.00	21.73
ATOM	143	N	ALA	174	56.123	32.461	7.716	1.00	19.69
ATOM	144	CA	ALA	174	55.844	33.155	8.968	1.00	18.07

ATOM	146	C	ALA	174	57.101	33.883	9.400	1.00	17.65
ATOM	147	O	ALA	174	57.052	35.031	9.829	1.00	19.80
ATOM	148	N	HIS	175	58.240	33.222	9.259	1.00	16.39
ATOM	149	CA	HIS	175	59.498	33.831	9.629	1.00	16.41
ATOM	150	CB	HIS	175	60.574	32.758	9.804	1.00	12.71
ATOM	151	CG	HIS	175	61.938	33.318	10.043	1.00	11.09
ATOM	152	CD2	HIS	175	62.373	34.252	10.920	1.00	8.26
ATOM	153	ND1	HIS	175	63.030	32.977	9.273	1.00	13.39
ATOM	154	CE1	HIS	175	64.076	33.683	9.658	1.00	13.77
ATOM	155	NE2	HIS	175	63.702	34.464	10.658	1.00	12.70
ATOM	156	C	HIS	175	59.959	34.903	8.624	1.00	19.55
ATOM	157	O	HIS	175	60.293	36.027	9.016	1.00	18.38
ATOM	158	N	ARG	176	59.987	34.555	7.339	1.00	20.77
ATOM	159	CA	ARG	176	60.424	35.494	6.307	1.00	21.30
ATOM	160	CB	ARG	176	60.315	34.876	4.917	1.00	24.87
ATOM	161	CG	ARG	176	61.361	33.827	4.609	1.00	30.22
ATOM	162	CD	ARG	176	61.429	33.603	3.116	1.00	36.29
ATOM	163	NE	ARG	176	62.256	32.457	2.758	1.00	44.72
ATOM	164	CZ	ARG	176	62.031	31.680	1.700	1.00	49.80
ATOM	165	NH1	ARG	176	61.000	31.935	0.894	1.00	50.83
ATOM	166	NH2	ARG	176	62.812	30.627	1.466	1.00	50.14
ATOM	167	C	ARG	176	59.658	36.807	6.337	1.00	20.67
ATOM	168	O	ARG	176	60.256	37.877	6.238	1.00	20.53
ATOM	169	N	SER	177	58.344	36.730	6.508	1.00	20.67
ATOM	170	CA	SER	177	57.526	37.934	6.551	1.00	21.86
ATOM	171	CB	SER	177	56.061	37.588	6.298	1.00	19.59
ATOM	172	OG	SER	177	55.541	36.774	7.329	1.00	21.85
ATOM	173	C	SER	177	57.659	38.733	7.857	1.00	23.27
ATOM	174	O	SER	177	57.073	39.807	7.989	1.00	24.40
ATOM	175	N	THR	178	58.383	38.202	8.837	1.00	22.16
ATOM	176	CA	THR	178	58.542	38.913	10.095	1.00	20.62
ATOM	177	CB	THR	178	57.853	38.162	11.265	1.00	19.93
ATOM	178	OG1	THR	178	58.386	36.838	11.381	1.00	18.72
ATOM	179	CG2	THR	178	56.359	38.057	11.033	1.00	16.95
ATOM	180	C	THR	178	60.015	39.137	10.394	1.00	21.57
ATOM	181	O	THR	178	60.368	39.649	11.449	1.00	23.91
ATOM	182	N	ASN	179	60.870	38.769	9.445	1.00	22.22
ATOM	183	CA	ASN	179	62.316	38.912	9.585	1.00	24.22
ATOM	184	CB	ASN	179	63.013	37.690	8.970	1.00	22.49
ATOM	185	CG	ASN	179	64.480	37.596	9.344	1.00	23.53
ATOM	186	OD1	ASN	179	64.866	37.912	10.464	1.00	22.32
ATOM	187	ND2	ASN	179	65.296	37.100	8.425	1.00	23.84
ATOM	188	C	ASN	179	62.744	40.210	8.881	1.00	26.52
ATOM	189	O	ASN	179	62.923	40.253	7.657	1.00	26.65
ATOM	190	N	ALA	180	62.898	41.267	9.671	1.00	27.47
ATOM	191	CA	ALA	180	63.255	42.582	9.166	1.00	30.30



ATOM	193	C	ALA	180	64.404	42.593	8.166	1.00	33.14	
ATOM	194	O	ALA	180	65.440	41.972	8.397	1.00	33.71	
ATOM	195	N	GLN	181	64.209	43.295	7.049	0.50	35.09	ALTA
ATOM	196	CA	GLN	181	65.212	43.423	5.980	0.50	37.44	ALTA
ATOM	197	CB	GLN	181	66.544	43.974	6.511	0.50	38.60	ALTA
ATOM	198	CG	GLN	181	66.728	45.462	6.299	0.50	40.53	ALTA
ATOM	199	CD	GLN	181	65.805	46.291	7.162	0.50	42.72	ALTA
ATOM	200	OE1	GLN	181	64.639	46.512	6.828	0.50	42.05	ALTA
ATOM	201	NE2	GLN	181	66.324	46.756	8.284	0.50	44.59	ALTA
ATOM	202	C	GLN	181	65.481	42.180	5.138	0.50	38.43	ALTA
ATOM	203	O	GLN	181	66.175	42.262	4.118	0.50	38.92	ALTA
ATOM	204	N	GLY	182	64.958	41.034	5.562	1.00	38.74	
ATOM	205	CA	GLY	182	65.166	39.808	4.805	1.00	40.07	
ATOM	206	C	GLY	182	66.634	39.554	4.486	1.00	42.06	
ATOM	207	O	GLY	182	67.504	39.684	5.346	1.00	43.28	
ATOM	208	N	SER	183	66.926	39.272	3.224	1.00	43.72	
ATOM	209	CA	SER	183	68.299	39.001	2.812	1.00	45.88	
ATOM	210	CB	SER	183	68.304	38.069	1.593	1.00	47.26	
ATOM	211	OG	SER	183	67.519	38.605	0.531	1.00	47.23	
ATOM	212	C	SER	183	69.095	40.268	2.497	1.00	46.24	
ATOM	213	O	SER	183	70.290	40.194	2.185	1.00	48.13	
ATOM	214	N	HIS	184	68.445	41.426	2.579	1.00	45.79	
ATOM	215	CA	HIS	184	69.111	42.690	2.276	1.00	45.00	
ATOM	216	CB	HIS	184	68.127	43.636	1.594	1.00	43.54	
ATOM	217	C	HIS	184	69.732	43.351	3.516	1.00	44.67	
ATOM	218	O	HIS	184	70.316	44.440	3.428	1.00	45.02	
ATOM	219	N	TRP	185	69.659	42.663	4.653	1.00	43.24	
ATOM	220	CA	TRP	185	70.190	43.172	5.919	1.00	40.98	
ATOM	221	CB	TRP	185	70.078	42.106	7.020	1.00	37.96	
ATOM	222	CG	TRP	185	70.889	40.874	6.775	1.00	34.14	
ATOM	223	CD2	TRP	185	72.197	40.593	7.291	1.00	33.38	
ATOM	224	CE2	TRP	185	72.572	39.321	6.807	1.00	31.68	
ATOM	225	CE3	TRP	185	73.092	41.296	8.107	1.00	31.65	
ATOM	226	CD1	TRP	185	70.530	39.790	6.028	1.00	34.27	
ATOM	227	NE1	TRP	185	71.536	38.852	6.043	1.00	33.51	
ATOM	228	CZ2	TRP	185	73.795	38.733	7.121	1.00	31.67	
ATOM	229	CZ3	TRP	185	74.308	40.713	8.419	1.00	31.29	
ATOM	230	CH2	TRP	185	74.651	39.444	7.923	1.00	31.06	
ATOM	231	C	TRP	185	71.618	43.720	5.856	1.00	41.52	
ATOM	232	O	TRP	185	71.893	44.817	6.335	1.00	40.52	
ATOM	233	N	LYS	186	72.520	42.976	5.234	1.00	42.94	
ATOM	234	CA	LYS	186	73.896	43.417	5.143	1.00	45.25	
ATOM	235	CB	LYS	186	74.764	42.328	4.508	1.00	45.96	
ATOM	236	CG	LYS	186	76.255</					



ATOM	240	C	LYS	186	74.025	44.730	4.377	1.00	47.38	
ATOM	241	O	LYS	186	74.914	45.535	4.663	1.00	47.65	
ATOM	242	N	GLN	187	73.134	44.959	3.418	0.50	48.02	ALTA
ATOM	243	CA	GLN	187	73.193	46.183	2.623	0.50	48.69	ALTA
ATOM	244	CB	GLN	187	72.547	45.973	1.246	0.50	48.66	ALTA
ATOM	245	CG	GLN	187	73.104	44.771	0.453	0.50	49.05	ALTA
ATOM	246	CD	GLN	187	74.624	44.766	0.339	0.50	49.17	ALTA
ATOM	247	OE1	GLN	187	75.225	45.691	-0.209	0.50	49.71	ALTA
ATOM	248	NE2	GLN	187	75.250	43.710	0.847	0.50	48.57	ALTA
ATOM	249	C	GLN	187	72.551	47.373	3.343	0.50	49.06	ALTA
ATOM	250	O	GLN	187	73.094	48.475	3.329	0.50	49.53	ALTA
ATOM	251	N	ARG	188	71.405	47.152	3.980	1.00	49.18	
ATOM	252	CA	ARG	188	70.723	48.221	4.695	1.00	49.90	
ATOM	253	CB	ARG	188	69.209	47.988	4.653	1.00	53.68	
ATOM	254	CG	ARG	188	68.617	47.798	3.251	1.00	57.22	
ATOM	255	CD	ARG	188	67.099	47.962	3.302	1.00	60.67	
ATOM	256	NE	ARG	188	66.430	47.441	2.110	1.00	64.43	
ATOM	257	CZ	ARG	188	65.931	46.208	2.009	1.00	66.13	
ATOM	258	NH1	ARG	188	66.027	45.362	3.031	1.00	66.69	
ATOM	259	NH2	ARG	188	65.318	45.823	0.893	1.00	66.10	
ATOM	260	C	ARG	188	71.150	48.510	6.133	1.00	48.42	
ATOM	261	O	ARG	188	70.544	49.368	6.784	1.00	48.86	
ATOM	262	N	ARG	189	72.153	47.804	6.647	1.00	46.00	
ATOM	263	CA	ARG	189	72.581	48.030	8.028	1.00	44.24	
ATOM	264	CB	ARG	189	73.039	46.726	8.690	1.00	43.40	
ATOM	265	CG	ARG	189	74.367	46.204	8.203	1.00	43.05	
ATOM	266	CD	ARG	189	74.808	45.021	9.019	1.00	43.62	
ATOM	267	NE	ARG	189	76.185	44.660	8.717	1.00	45.95	
ATOM	268	CZ	ARG	189	76.981	43.976	9.536	1.00	48.56	
ATOM	269	NH1	ARG	189	76.548	43.560	10.724	1.00	46.34	
ATOM	270	NH2	ARG	189	78.233	43.735	9.174	1.00	50.12	
ATOM	271	C	ARG	189	73.642	49.116	8.238	1.00	43.20	
ATOM	272	O	ARG	189	74.629	49.210	7.500	1.00	43.07	
ATOM	273	N	LYS	190	73.427	49.925	9.268	1.00	41.56	
ATOM	274	CA	LYS	190	74.335	51.003	9.628	1.00	39.96	
ATOM	275	CB	LYS	190	73.563	52.323	9.757	1.00	38.85	
ATOM	276	C	LYS	190	74.983	50.631	10.956	1.00	38.91	
ATOM	277	O	LYS	190	74.345	50.015	11.806	1.00	38.17	
ATOM	278	N	PHE	191	76.261	50.959	11.104	1.00	38.49	
ATOM	279	CA	PHE	191	76.998	50.673	12.326	1.00	38.42	
ATOM	280	CB	PHE	191	78.500	50.762	12.073	1.00	38.37	
ATOM	281	CG	PHE	191	79.056	49.608	11.308	1.00	39.05	
ATOM	282	CD1	PHE	191	78.712	49.408	9.976	1.00	40.02	
ATOM	283	CD2	PHE	191	79.942	48.				

ATOM	287	C	PHE	191	76.650	51.673	13.416	1.00	37.96
ATOM	288	O	PHE	191	76.568	52.872	13.151	1.00	38.95
ATOM	289	N	LEU	192	76.433	51.184	14.634	1.00	37.05
ATOM	290	CA	LEU	192	76.138	52.063	15.759	1.00	35.99
ATOM	291	CB	LEU	192	75.833	51.247	17.014	1.00	33.04
ATOM	292	CG	LEU	192	75.503	52.074	18.260	1.00	31.38
ATOM	293	CD1	LEU	192	74.116	52.651	18.102	1.00	29.02
ATOM	294	CD2	LEU	192	75.592	51.229	19.536	1.00	30.32
ATOM	295	C	LEU	192	77.436	52.831	15.976	1.00	36.99
ATOM	296	O	LEU	192	78.500	52.218	16.112	1.00	37.66
ATOM	297	N	PRO	193	77.377	54.177	15.988	1.00	38.15
ATOM	298	CD	PRO	193	76.156	54.996	15.902	1.00	37.90
ATOM	299	CA	PRO	193	78.561	55.025	16.187	1.00	38.68
ATOM	300	CB	PRO	193	77.950	56.365	16.568	1.00	37.20
ATOM	301	CG	PRO	193	76.711	56.397	15.758	1.00	37.08
ATOM	302	C	PRO	193	79.475	54.503	17.294	1.00	41.12
ATOM	303	O	PRO	193	79.005	54.129	18.367	1.00	42.26
ATOM	304	N	ASP	194	80.782	54.509	17.052	1.00	43.62
ATOM	305	CA	ASP	194	81.731	54.012	18.050	1.00	46.71
ATOM	306	CB	ASP	194	83.131	53.938	17.470	1.00	49.32
ATOM	307	CG	ASP	194	83.237	52.904	16.397	1.00	52.34
ATOM	308	OD1	ASP	194	83.539	51.726	16.719	1.00	53.18
ATOM	309	OD2	ASP	194	82.981	53.268	15.227	1.00	55.10
ATOM	310	C	ASP	194	81.769	54.743	19.386	1.00	47.12
ATOM	311	O	ASP	194	82.158	54.163	20.403	1.00	48.16
ATOM	312	N	ASP	195	81.389	56.015	19.386	1.00	47.54
ATOM	313	CA	ASP	195	81.382	56.791	20.620	1.00	48.68
ATOM	314	CB	ASP	195	81.180	58.285	20.322	1.00	50.76
ATOM	315	CG	ASP	195	79.871	58.572	19.602	1.00	54.24
ATOM	316	OD1	ASP	195	78.929	59.082	20.253	1.00	56.17
ATOM	317	OD2	ASP	195	79.786	58.292	18.385	1.00	56.08
ATOM	318	C	ASP	195	80.304	56.274	21.580	1.00	47.63
ATOM	319	O	ASP	195	80.294	56.621	22.772	1.00	49.07
ATOM	320	N	ILE	196	79.400	55.444	21.065	1.00	44.87
ATOM	321	CA	ILE	196	78.330	54.890	21.888	1.00	42.53
ATOM	322	CB	ILE	196	76.983	54.813	21.121	1.00	42.19
ATOM	323	CG2	ILE	196	75.870	54.357	22.060	1.00	40.29
ATOM	324	CG1	ILE	196	76.635	56.191	20.535	1.00	41.32
ATOM	325	CD1	ILE	196	75.344	56.219	19.732	1.00	41.32
ATOM	326	C	ILE	196	78.725	53.509	22.391	1.00	40.89
ATOM	327	O	ILE	196	79.358	52.722	21.679	1.00	40.08
ATOM	328	N	GLY	197	78.384	53.240	23.642	1.00	40.16
ATOM	329	CA	GLY	197	78.705	51.957	24.228	1.00	40.21
ATOM	330	C	GLY	197	80.066	51.907	24.879	1.00	40.18
ATOM	331	O	GLY	197	80.512	50.839	25.267	1.00	40.55
ATOM	332	N	GLN	198	80.71				

ATOM	334	CB	GLN	198	83.041	53.823	24.738	1.00	39.51
ATOM	335	C	GLN	198	81.995	53.796	27.046	1.00	40.93
ATOM	336	O	GLN	198	83.036	54.197	27.571	1.00	41.83
ATOM	337	N	SER	199	80.806	53.859	27.654	1.00	39.68
ATOM	338	CA	SER	199	80.615	54.510	28.961	1.00	37.74
ATOM	339	CB	SER	199	79.995	55.905	28.768	1.00	38.50
ATOM	340	OG	SER	199	80.687	56.672	27.792	1.00	40.71
ATOM	341	C	SER	199	79.743	53.726	29.958	1.00	36.31
ATOM	342	O	SER	199	78.719	54.228	30.436	1.00	35.69
ATOM	343	N	PRO	200	80.123	52.484	30.280	1.00	35.05
ATOM	344	CD	PRO	200	81.246	51.684	29.760	1.00	33.97
ATOM	345	CA	PRO	200	79.313	51.715	31.228	1.00	35.89
ATOM	346	CB	PRO	200	79.872	50.304	31.075	1.00	33.94
ATOM	347	CG	PRO	200	81.297	50.532	30.708	1.00	33.31
ATOM	348	C	PRO	200	79.477	52.241	32.656	1.00	37.75
ATOM	349	O	PRO	200	80.484	51.959	33.299	1.00	38.78
ATOM	350	N	ILE	201	78.493	52.988	33.158	1.00	39.61
ATOM	351	CA	ILE	201	78.590	53.551	34.511	1.00	40.56
ATOM	352	CB	ILE	201	78.715	55.093	34.484	1.00	40.20
ATOM	353	CG2	ILE	201	80.125	55.501	34.082	1.00	41.06
ATOM	354	CG1	ILE	201	77.690	55.694	33.532	1.00	40.98
ATOM	355	CD1	ILE	201	77.969	57.147	33.205	1.00	44.31
ATOM	356	C	ILE	201	77.535	53.160	35.546	1.00	41.40
ATOM	357	O	ILE	201	77.768	53.313	36.751	1.00	42.09
ATOM	358	N	VAL	202	76.365	52.701	35.104	1.00	41.42
ATOM	359	CA	VAL	202	75.325	52.293	36.053	1.00	40.70
ATOM	360	CB	VAL	202	73.913	52.292	35.422	1.00	38.44
ATOM	361	CG1	VAL	202	72.881	51.826	36.435	1.00	35.91
ATOM	362	CG2	VAL	202	73.560	53.692	34.934	1.00	36.42
ATOM	363	C	VAL	202	75.687	50.917	36.622	1.00	41.64
ATOM	364	O	VAL	202	76.094	50.008	35.894	1.00	42.05
ATOM	365	N	SER	203	75.596	50.800	37.938	1.00	43.06
ATOM	366	CA	SER	203	75.947	49.576	38.639	1.00	44.57
ATOM	367	CB	SER	203	75.916	49.842	40.154	1.00	46.82
ATOM	368	OG	SER	203	76.457	48.772	40.916	1.00	50.18
ATOM	369	C	SER	203	75.052	48.388	38.294	1.00	44.08
ATOM	370	O	SER	203	73.849	48.534	38.093	1.00	44.28
ATOM	371	N	MET	204	75.656	47.210	38.231	1.00	43.11
ATOM	372	CA	MET	204	74.930	45.980	37.963	1.00	43.12
ATOM	373	CB	MET	204	75.048	45.557	36.494	1.00	41.07
ATOM	374	CG	MET	204	74.126	46.320	35.554	1.00	36.96
ATOM	375	SD	MET	204	72.375	46.134	35.990	1.00	38.66
ATOM	376	CE	MET	204	71.970	44.592	35.098	1.00	37.26
ATOM	377	C	MET	204	75.561	44.943	38.866	1.00	43.68
ATOM	378	O	MET	204	76.784	44.817	38.912	1.00	44.32
ATOM	379	N	PRO	205	74.735	44.204	39.619	1.00	44.22
ATOM	380	CD	PRO	205	73.261	44.310	39.610	1.00	44.44

ATOM	381	CA	PRO	205	75.187	43.164	40.546	1.00	44.32
ATOM	382	CB	PRO	205	73.944	42.299	40.701	1.00	45.18
ATOM	383	CG	PRO	205	72.832	43.335	40.691	1.00	44.29
ATOM	384	C	PRO	205	76.417	42.354	40.122	1.00	44.31
ATOM	385	O	PRO	205	77.393	42.293	40.864	1.00	43.97
ATOM	386	N <sup>-</sup>	ASP	206	76.404	41.802	38.912	1.00	44.30
ATOM	387	CA	ASP	206	77.524	40.984	38.433	1.00	44.77
ATOM	388	CB	ASP	206	77.073	40.106	37.270	1.00	47.12
ATOM	389	CG	ASP	206	76.503	40.912	36.120	1.00	49.73
ATOM	390	OD1	ASP	206	76.992	42.039	35.863	1.00	49.65
ATOM	391	OD2	ASP	206	75.553	40.416	35.478	1.00	51.96
ATOM	392	C	ASP	206	78.805	41.718	38.037	1.00	44.10
ATOM	393	O	ASP	206	79.754	41.099	37.549	1.00	43.60
ATOM	394	N	GLY	207	78.804	43.039	38.145	1.00	44.19
ATOM	395	CA	GLY	207	80.001	43.785	37.803	1.00	43.51
ATOM	396	C	GLY	207	80.041	44.425	36.433	1.00	43.29
ATOM	397	O	GLY	207	80.745	45.421	36.257	1.00	44.47
ATOM	398	N	ASP	208	79.363	43.845	35.446	1.00	42.45
ATOM	399	CA	ASP	208	79.347	44.436	34.106	1.00	41.51
ATOM	400	CB	ASP	208	78.915	43.402	33.070	1.00	42.91
ATOM	401	CG	ASP	208	80.001	42.379	32.785	1.00	43.57
ATOM	402	OD1	ASP	208	79.675	41.218	32.468	1.00	44.55
ATOM	403	OD2	ASP	208	81.191	42.742	32.868	1.00	47.14
ATOM	404	C	ASP	208	78.378	45.606	34.143	1.00	40.78
ATOM	405	O	ASP	208	77.176	45.403	34.277	1.00	42.50
ATOM	406	N	LYS	209	78.902	46.827	34.058	1.00	39.10
ATOM	407	CA	LYS	209	78.071	48.033	34.150	1.00	37.23
ATOM	408	CB	LYS	209	78.910	49.211	34.681	1.00	37.29
ATOM	409	C	LYS	209	77.326	48.423	32.871	1.00	34.47
ATOM	410	O	LYS	209	77.707	48.013	31.776	1.00	33.85
ATOM	411	N	VAL	210	76.275	49.228	33.028	1.00	33.30
ATOM	412	CA	VAL	210	75.448	49.684	31.907	1.00	31.78
ATOM	413	CB	VAL	210	73.929	49.618	32.235	1.00	29.51
ATOM	414	CG1	VAL	210	73.102	50.012	31.010	1.00	29.24
ATOM	415	CG2	VAL	210	73.541	48.237	32.698	1.00	29.84
ATOM	416	C	VAL	210	75.731	51.115	31.451	1.00	32.68
ATOM	417	O	VAL	210	75.845	52.033	32.264	1.00	32.69
ATOM	418	N	ASP	211	75.769	51.290	30.134	1.00	33.00
ATOM	419	CA	ASP	211	75.978	52.574	29.476	1.00	31.85
ATOM	420	CB	ASP	211	76.826	52.353	28.221	1.00	32.38
ATOM	421	CG	ASP	211	77.019	53.612	27.386	1.00	31.88
ATOM	422	OD1	ASP	211	78.123	53.768	26.843	1.00	32.78
ATOM	423	OD2	ASP	211	76.079	54.412	27.208	1.00	32.32
ATOM	424	C	ASP	211	74.562	53.023	29.101	1.00	33.39
ATOM	425	O	ASP	211	73.925	52.444	28.206	1.00	31.94
ATOM	426	N	LEU	212	74.078	54.063	29.770	1.00	32.50
ATOM	427	CA	LEU	212	72.731	54.568	29.532	1.00	32.29



ATOM	428	CB	LEU	212	72.440	55.736	30.470	1.00	32.41
ATOM	429	CG	LEU	212	72.311	55.336	31.936	1.00	32.11
ATOM	430	CD1	LEU	212	72.447	56.555	32.830	1.00	32.35
ATOM	431	CD2	LEU	212	70.979	54.650	32.148	1.00	30.87
ATOM	432	C	LEU	212	72.419	54.962	28.092	1.00	32.29
ATOM	433	O-	LEU	212	71.326	54.695	27.609	1.00	32.13
ATOM	434	N	GLU	213	73.370	55.589	27.407	1.00	32.21
ATOM	435	CA	GLU	213	73.144	56.007	26.028	1.00	33.12
ATOM	436	CB	GLU	213	74.305	56.864	25.530	1.00	36.72
ATOM	437	CG	GLU	213	74.067	57.468	24.146	1.00	40.61
ATOM	438	CD	GLU	213	75.316	58.101	23.545	1.00	44.21
ATOM	439	OE1	GLU	213	76.434	57.851	24.059	1.00	46.23
ATOM	440	OE2	GLU	213	75.178	58.836	22.543	1.00	45.81
ATOM	441	C	GLU	213	72.966	54.801	25.111	1.00	31.91
ATOM	442	O	GLU	213	72.064	54.775	24.273	1.00	31.31
ATOM	443	N	ALA	214	73.827	53.803	25.285	1.00	30.66
ATOM	444	CA	ALA	214	73.769	52.585	24.482	1.00	30.43
ATOM	445	CB	ALA	214	74.971	51.690	24.783	1.00	29.77
ATOM	446	C	ALA	214	72.464	51.854	24.778	1.00	29.34
ATOM	447	O	ALA	214	71.772	51.421	23.862	1.00	28.33
ATOM	448	N	PHE	215	72.116	51.762	26.058	1.00	28.45
ATOM	449	CA	PHE	215	70.882	51.116	26.492	1.00	29.05
ATOM	450	CB	PHE	215	70.732	51.240	28.005	1.00	25.98
ATOM	451	CG	PHE	215	69.443	50.689	28.535	1.00	25.53
ATOM	452	CD1	PHE	215	69.330	49.344	28.854	1.00	26.16
ATOM	453	CD2	PHE	215	68.349	51.519	28.737	1.00	25.04
ATOM	454	CE1	PHE	215	68.144	48.831	29.370	1.00	25.73
ATOM	455	CE2	PHE	215	67.160	51.018	29.252	1.00	25.84
ATOM	456	CZ	PHE	215	67.058	49.669	29.570	1.00	25.25
ATOM	457	C	PHE	215	69.694	51.780	25.801	1.00	30.92
ATOM	458	O	PHE	215	68.773	51.107	25.316	1.00	30.38
ATOM	459	N	SER	216	69.714	53.108	25.776	1.00	31.41
ATOM	460	CA	SER	216	68.667	53.887	25.136	1.00	31.23
ATOM	461	CB	SER	216	68.976	55.375	25.256	1.00	32.50
ATOM	462	OG	SER	216	67.972	56.153	24.628	1.00	35.83
ATOM	463	C	SER	216	68.600	53.504	23.663	1.00	31.67
ATOM	464	O	SER	216	67.527	53.235	23.129	1.00	31.34
ATOM	465	N	GLU	217	69.756	53.475	23.014	1.00	31.72
ATOM	466	CA	GLU	217	69.823	53.121	21.609	1.00	33.06
ATOM	467	CB	GLU	217	71.269	53.153	21.110	1.00	34.93
ATOM	468	CG	GLU	217	71.824	54.557	20.921	1.00	38.98
ATOM	469	CD	GLU	217	70.986	55.399	19.963	1.00	41.92
ATOM	470	OE1	GLU	217	70.177	56.221	20.444	1.00	44.02
ATOM	471	OE2	GLU	217	71.139	55.246	18.731	1.00	44.46
ATOM	472	C	GLU	217	69.199	51.759	21.330	1.00	31.78
ATOM	473	O	GLU						



ATOM	475	CA	PHE	218	68.924	49.447	21.979	1.00	27.65
ATOM	476	CB	PHE	218	69.668	48.416	22.827	1.00	26.79
ATOM	477	CG	PHE	218	71.114	48.292	22.467	1.00	24.76
ATOM	478	CD1	PHE	218	72.083	48.191	23.446	1.00	24.37
ATOM	479	CD2	PHE	218	71.510	48.354	21.134	1.00	24.30
ATOM	480	CE1	PHE	218	73.424	48.167	23.106	1.00	23.85
ATOM	481	CE2	PHE	218	72.843	48.329	20.785	1.00	23.07
ATOM	482	CZ	PHE	218	73.804	48.236	21.772	1.00	24.45
ATOM	483	C	PHE	218	67.441	49.403	22.255	1.00	26.94
ATOM	484	O	PHE	218	66.658	48.985	21.409	1.00	27.98
ATOM	485	N	THR	219	67.032	49.906	23.405	1.00	26.97
ATOM	486	CA	THR	219	65.619	49.876	23.740	1.00	27.25
ATOM	487	CB	THR	219	65.379	50.304	25.195	1.00	27.35
ATOM	488	OG1	THR	219	65.924	51.612	25.410	1.00	26.48
ATOM	489	CG2	THR	219	66.034	49.303	26.139	1.00	24.51
ATOM	490	C	THR	219	64.747	50.689	22.782	1.00	27.21
ATOM	491	O	THR	219	63.588	50.348	22.557	1.00	28.58
ATOM	492	N	LYS	220	65.318	51.726	22.184	1.00	26.75
ATOM	493	CA	LYS	220	64.576	52.569	21.254	1.00	27.81
ATOM	494	CB	LYS	220	65.439	53.753	20.782	1.00	27.46
ATOM	495	C	LYS	220	64.058	51.772	20.056	1.00	28.62
ATOM	496	O	LYS	220	63.014	52.101	19.500	1.00	28.63
ATOM	497	N	ILE	221	64.774	50.721	19.662	1.00	28.92
ATOM	498	CA	ILE	221	64.331	49.907	18.527	1.00	28.19
ATOM	499	CB	ILE	221	65.450	49.732	17.465	1.00	27.17
ATOM	500	CG2	ILE	221	65.866	51.095	16.911	1.00	26.61
ATOM	501	CG1	ILE	221	66.645	48.977	18.061	1.00	26.80
ATOM	502	CD1	ILE	221	67.621	48.417	17.029	1.00	24.91
ATOM	503	C	ILE	221	63.840	48.512	18.937	1.00	28.82
ATOM	504	O	ILE	221	63.552	47.678	18.076	1.00	28.59
ATOM	505	N	ILE	222	63.690	48.263	20.236	1.00	27.09
ATOM	506	CA	ILE	222	63.279	46.934	20.665	1.00	27.22
ATOM	507	CB	ILE	222	63.777	46.591	22.101	1.00	26.58
ATOM	508	CG2	ILE	222	62.815	47.151	23.171	1.00	23.83
ATOM	509	CG1	ILE	222	63.949	45.065	22.230	1.00	24.15
ATOM	510	CD1	ILE	222	64.727	44.610	23.458	1.00	21.43
ATOM	511	C	ILE	222	61.797	46.614	20.519	1.00	28.33
ATOM	512	O	ILE	222	61.445	45.459	20.260	1.00	29.81
ATOM	513	N	THR	223	60.929	47.618	20.622	1.00	27.63
ATOM	514	CA	THR	223	59.494	47.366	20.505	1.00	26.83
ATOM	515	CB	THR	223	58.667	48.631	20.797	1.00	29.85
ATOM	516	OG1	THR	223	58.839	48.983	22.180	1.00	30.67
ATOM	517	CG2	THR	223	57.183	48.390	20.525	1.00	26.50
ATOM	518	C	THR	223	59.103	46.698	19.183	1.00	25.28
ATOM	519	O	THR	223	58.390	45.691	19.196	1.00	24.87
ATOM	520	N	PRO	224	59.535	47.256	18.031	1.00	23.96
ATOM	521	CD	PRO	224	60.138	48.580	17.792	1.00	22.28

ATOM	522	CA	PRO	224	59.181	46.612	16.759	1.00	23.13
ATOM	523	CB	PRO	224	59.747	47.570	15.699	1.00	22.96
ATOM	524	CG	PRO	224	60.762	48.406	16.443	1.00	24.53
ATOM	525	C	PRO	224	59.790	45.204	16.634	1.00	22.56
ATOM	526	O	PRO	224	59.198	44.332	15.994	1.00	22.77
ATOM	527	N	ALA	225	60.960	44.989	17.240	1.00	19.17
ATOM	528	CA	ALA	225	61.622	43.684	17.213	1.00	18.54
ATOM	529	CB	ALA	225	63.009	43.773	17.806	1.00	16.79
ATOM	530	C	ALA	225	60.802	42.643	17.969	1.00	19.08
ATOM	531	O	ALA	225	60.681	41.502	17.523	1.00	21.30
ATOM	532	N	ILE	226	60.253	43.033	19.117	1.00	18.30
ATOM	533	CA	ILE	226	59.420	42.147	19.929	1.00	18.65
ATOM	534	CB	ILE	226	59.092	42.779	21.288	1.00	17.30
ATOM	535	CG2	ILE	226	58.057	41.952	22.020	1.00	17.76
ATOM	536	CG1	ILE	226	60.361	42.915	22.123	1.00	17.07
ATOM	537	CD1	ILE	226	60.175	43.775	23.351	1.00	14.65
ATOM	538	C	ILE	226	58.109	41.858	19.199	1.00	19.56
ATOM	539	O	ILE	226	57.638	40.719	19.163	1.00	19.51
ATOM	540	N	THR	227	57.521	42.903	18.627	1.00	20.26
ATOM	541	CA	THR	227	56.278	42.782	17.881	1.00	21.19
ATOM	542	CB	THR	227	55.856	44.150	17.326	1.00	22.41
ATOM	543	OG1	THR	227	55.670	45.053	18.420	1.00	25.09
ATOM	544	CG2	THR	227	54.558	44.041	16.560	1.00	24.29
ATOM	545	C	THR	227	56.411	41.758	16.742	1.00	20.16
ATOM	546	O	THR	227	55.487	40.978	16.496	1.00	21.18
ATOM	547	N	ARG	228	57.558	41.744	16.069	1.00	18.42
ATOM	548	CA	ARG	228	57.783	40.786	14.991	1.00	18.29
ATOM	549	CB	ARG	228	59.032	41.136	14.191	1.00	19.95
ATOM	550	CG	ARG	228	58.810	42.349	13.286	1.00	23.31
ATOM	551	CD	ARG	228	60.001	42.646	12.405	1.00	25.64
ATOM	552	NE	ARG	228	61.139	43.138	13.171	1.00	27.01
ATOM	553	CZ	ARG	228	62.209	42.413	13.468	1.00	28.20
ATOM	554	NH1	ARG	228	62.280	41.155	13.067	1.00	28.99
ATOM	555	NH2	ARG	228	63.219	42.951	14.141	1.00	27.25
ATOM	556	C	ARG	228	57.834	39.352	15.502	1.00	18.40
ATOM	557	O	ARG	228	57.433	38.431	14.788	1.00	17.50
ATOM	558	N	VAL	229	58.278	39.162	16.747	1.00	17.42
ATOM	559	CA	VAL	229	58.316	37.822	17.334	1.00	16.40
ATOM	560	CB	VAL	229	59.116	37.779	18.674	1.00	15.88
ATOM	561	CG1	VAL	229	58.955	36.422	19.334	1.00	16.19
ATOM	562	CG2	VAL	229	60.591	38.010	18.421	1.00	14.44
ATOM	563	C	VAL	229	56.852	37.408	17.552	1.00	16.75
ATOM	564	O	VAL	229	56.456	36.282	17.219	1.00	16.06
ATOM	565	N	VAL	230	56.039	38.343	18.046	1.00	16.09
ATOM	566	CA	VAL	230	54.612	38.097	18.266	1.00	16.97
ATOM	567	CB	VAL	230	53.896	39.3			

ATOM	569	CG2 VAL	230	54.445	39.629	20.299	1.00	17.82
ATOM	570	C VAL	230	53.938	37.780	16.916	1.00	18.46
ATOM	571	O VAL	230	53.115	36.863	16.828	1.00	18.46
ATOM	572	N ASP	231	54.289	38.539	15.874	1.00	19.21
ATOM	573	CA ASP	231	53.730	38.339	14.531	1.00	19.93
ATOM	574	CB ASP	231	54.231	39.415	13.555	1.00	20.98
ATOM	575	CG ASP	231	53.754	40.817	13.915	1.00	24.11
ATOM	576	OD1 ASP	231	52.704	40.953	14.586	1.00	24.23
ATOM	577	OD2 ASP	231	54.443	41.784	13.522	1.00	25.90
ATOM	578	C ASP	231	54.097	36.962	13.982	1.00	19.27
ATOM	579	O ASP	231	53.266	36.279	13.380	1.00	17.80
ATOM	580	N PHE	232	55.357	36.582	14.163	1.00	18.91
ATOM	581	CA PHE	232	55.841	35.288	13.712	1.00	19.65
ATOM	582	CB PHE	232	57.308	35.078	14.104	1.00	18.14
ATOM	583	CG PHE	232	57.752	33.639	14.027	1.00	19.70
ATOM	584	CD1 PHE	232	57.895	33.005	12.799	1.00	19.18
ATOM	585	CD2 PHE	232	57.987	32.904	15.188	1.00	17.61
ATOM	586	CE1 PHE	232	58.259	31.660	12.723	1.00	19.86
ATOM	587	CE2 PHE	232	58.350	31.560	15.126	1.00	18.98
ATOM	588	CZ PHE	232	58.487	30.935	13.892	1.00	19.46
ATOM	589	C PHE	232	54.996	34.179	14.320	1.00	21.02
ATOM	590	O PHE	232	54.458	33.339	13.598	1.00	20.88
ATOM	591	N ALA	233	54.863	34.202	15.645	1.00	21.64
ATOM	592	CA ALA	233	54.106	33.187	16.378	1.00	21.43
ATOM	593	CB ALA	233	54.223	33.443	17.868	1.00	18.72
ATOM	594	C ALA	233	52.643	33.134	15.955	1.00	23.15
ATOM	595	O ALA	233	52.043	32.062	15.857	1.00	21.76
ATOM	596	N LYS	234	52.083	34.307	15.689	1.00	25.54
ATOM	597	CA LYS	234	50.695	34.446	15.273	1.00	27.57
ATOM	598	CB LYS	234	50.360	35.935	15.146	1.00	30.65
ATOM	599	CG LYS	234	49.110	36.349	15.867	1.00	36.27
ATOM	600	CD LYS	234	49.192	35.988	17.334	1.00	41.19
ATOM	601	CE LYS	234	47.800	35.677	17.890	1.00	43.69
ATOM	602	NZ LYS	234	47.119	34.565	17.147	1.00	44.98
ATOM	603	C LYS	234	50.443	33.739	13.933	1.00	27.70
ATOM	604	O LYS	234	49.355	33.200	13.693	1.00	28.42
ATOM	605	N LYS	235	51.458	33.732	13.074	1.00	26.06
ATOM	606	CA LYS	235	51.364	33.113	11.758	1.00	26.47
ATOM	607	CB LYS	235	52.350	33.791	10.819	1.00	25.23
ATOM	608	CG LYS	235	52.051	35.269	10.644	1.00	26.92
ATOM	609	CD LYS	235	53.017	35.959	9.697	1.00	28.41
ATOM	610	CE LYS	235	52.500	37.350	9.318	1.00	29.31
ATOM	611	NZ LYS	235	53.400	38.026	8.347	1.00	30.37
ATOM	612	C LYS	235	51.540	31.588	11.722	1.00	27.93
ATOM	613	O LYS	235	51.540	30.984	10.649	1.00	29.04
ATOM	614	N LEU	236	51.718	30.973	12.887	1.00	28.83
ATOM	615	CA LEU	236	51.866	29.524	12.986	1.00	29.05

ATOM	616	CB	LEU	236	52.928	29.150	14.026	1.00	27.43
ATOM	617	CG	LEU	236	54.352	29.660	13.774	1.00	25.84
ATOM	618	CD1	LEU	236	55.311	29.118	14.847	1.00	23.99
ATOM	619	CD2	LEU	236	54.801	29.236	12.389	1.00	23.86
ATOM	620	C	LEU	236	50.513	28.948	13.392	1.00	31.19
ATOM	621	O <sup>-</sup>	LEU	236	49.870	29.435	14.328	1.00	31.48
ATOM	622	N	PRO	237	50.078	27.875	12.717	1.00	34.60
ATOM	623	CD	PRO	237	50.829	27.156	11.668	1.00	35.04
ATOM	624	CA	PRO	237	48.789	27.223	13.002	1.00	36.52
ATOM	625	CB	PRO	237	48.751	26.081	11.981	1.00	37.48
ATOM	626	CG	PRO	237	50.229	25.776	11.718	1.00	36.60
ATOM	627	C	PRO	237	48.582	26.720	14.447	1.00	37.82
ATOM	628	O	PRO	237	47.629	27.102	15.125	1.00	37.08
ATOM	629	N	MET	238	49.495	25.893	14.935	1.00	40.42
ATOM	630	CA	MET	238	49.366	25.350	16.285	1.00	43.00
ATOM	631	CB	MET	238	50.453	24.298	16.549	1.00	45.20
ATOM	632	CG	MET	238	50.043	22.837	16.296	1.00	47.16
ATOM	633	SD	MET	238	50.598	22.117	14.725	1.00	52.25
ATOM	634	CE	MET	238	52.305	21.809	15.033	1.00	47.29
ATOM	635	C	MET	238	49.389	26.389	17.414	1.00	43.25
ATOM	636	O	MET	238	49.061	26.056	18.558	1.00	44.74
ATOM	637	N	PHE	239	49.720	27.642	17.088	1.00	41.55
ATOM	638	CA	PHE	239	49.825	28.716	18.091	1.00	37.31
ATOM	639	CB	PHE	239	51.031	29.615	17.765	1.00	32.40
ATOM	640	CG	PHE	239	51.293	30.673	18.795	1.00	27.12
ATOM	641	CD1	PHE	239	52.099	30.398	19.893	1.00	24.57
ATOM	642	CD2	PHE	239	50.705	31.933	18.686	1.00	24.70
ATOM	643	CE1	PHE	239	52.319	31.356	20.876	1.00	25.09
ATOM	644	CE2	PHE	239	50.915	32.901	19.659	1.00	25.90
ATOM	645	CZ	PHE	239	51.726	32.612	20.761	1.00	24.52
ATOM	646	C	PHE	239	48.574	29.582	18.352	1.00	36.84
ATOM	647	O	PHE	239	48.136	29.728	19.497	1.00	34.67
ATOM	648	N	SER	240	48.027	30.180	17.299	1.00	36.92
ATOM	649	CA	SER	240	46.857	31.038	17.433	1.00	37.16
ATOM	650	CB	SER	240	46.534	31.706	16.094	1.00	38.34
ATOM	651	C	SER	240	45.627	30.304	17.981	1.00	37.30
ATOM	652	O	SER	240	44.680	30.941	18.433	1.00	36.95
ATOM	653	N	GLU	241	45.639	28.974	17.917	1.00	37.73
ATOM	654	CA	GLU	241	44.531	28.155	18.418	1.00	38.44
ATOM	655	CB	GLU	241	44.644	26.705	17.912	1.00	42.18
ATOM	656	CG	GLU	241	44.290	26.471	16.436	1.00	48.01
ATOM	657	CD	GLU	241	44.559	25.028	15.973	1.00	50.12
ATOM	658	OE1	GLU	241	44.375	24.088	16.779	1.00	51.14
ATOM	659	OE2	GLU	241	44.957	24.838	14.799	1.00	50.68
ATOM	660	C	GLU	241	44.571	28.122	19.937	1.00	35.85
ATOM	661	O	GLU	241					



ATOM	663	CA	LEU	242	45.959	28.296	21.920	1.00	31.31
ATOM	664	CB	LEU	242	47.452	28.382	22.244	1.00	29.28
ATOM	665	CG	LEU	242	48.318	27.202	21.797	1.00	29.95
ATOM	666	CD1	LEU	242	49.771	27.538	22.025	1.00	29.19
ATOM	667	CD2	LEU	242	47.935	25.931	22.564	1.00	29.57
ATOM	668	C <sup>-</sup>	LEU	242	45.223	29.390	22.676	1.00	30.10
ATOM	669	O	LEU	242	44.874	30.434	22.116	1.00	28.69
ATOM	670	N	PRO	243	44.867	29.115	23.937	1.00	30.09
ATOM	671	CD	PRO	243	44.783	27.843	24.674	1.00	28.53
ATOM	672	CA	PRO	243	44.183	30.200	24.640	1.00	31.01
ATOM	673	CB	PRO	243	43.829	29.577	26.005	1.00	30.34
ATOM	674	CG	PRO	243	44.640	28.300	26.093	1.00	29.25
ATOM	675	C	PRO	243	45.195	31.356	24.774	1.00	31.71
ATOM	676	O	PRO	243	46.412	31.128	24.840	1.00	30.69
ATOM	677	N	CYS	244	44.694	32.585	24.804	1.00	32.36
ATOM	678	CA	CYS	244	45.539	33.763	24.920	1.00	33.57
ATOM	679	CB	CYS	244	44.675	35.028	25.050	1.00	37.62
ATOM	680	SG	CYS	244	45.262	36.418	24.022	1.00	51.95
ATOM	681	C	CYS	244	46.536	33.660	26.081	1.00	31.12
ATOM	682	O	CYS	244	47.677	34.087	25.942	1.00	30.37
ATOM	683	N	GLU	245	46.124	33.045	27.194	1.00	30.00
ATOM	684	CA	GLU	245	46.993	32.877	28.366	1.00	29.62
ATOM	685	CB	GLU	245	46.270	32.159	29.514	1.00	33.10
ATOM	686	CG	GLU	245	45.325	33.018	30.333	1.00	36.43
ATOM	687	CD	GLU	245	43.882	32.940	29.860	1.00	37.87
ATOM	688	OE1	GLU	245	42.989	33.006	30.730	1.00	37.36
ATOM	689	OE2	GLU	245	43.639	32.813	28.634	1.00	39.63
ATOM	690	C	GLU	245	48.239	32.077	28.030	1.00	28.34
ATOM	691	O	GLU	245	49.322	32.343	28.557	1.00	27.88
ATOM	692	N	ASP	246	48.063	31.043	27.213	1.00	26.10
ATOM	693	CA	ASP	246	49.182	30.212	26.798	1.00	25.23
ATOM	694	CB	ASP	246	48.685	28.923	26.135	1.00	26.98
ATOM	695	CG	ASP	246	48.146	27.912	27.137	1.00	29.13
ATOM	696	OD1	ASP	246	48.158	28.193	28.354	1.00	26.52
ATOM	697	OD2	ASP	246	47.712	26.824	26.696	1.00	31.38
ATOM	698	C	ASP	246	50.065	30.983	25.826	1.00	23.57
ATOM	699	O	ASP	246	51.288	30.993	25.955	1.00	22.61
ATOM	700	N	GLN	247	49.431	31.630	24.852	1.00	23.23
ATOM	701	CA	GLN	247	50.144	32.408	23.855	1.00	22.20
ATOM	702	CB	GLN	247	49.159	33.178	22.991	1.00	22.06
ATOM	703	CG	GLN	247	48.329	32.307	22.066	1.00	22.74
ATOM	704	CD	GLN	247	47.435	33.141	21.169	1.00	24.91
ATOM	705	OE1	GLN	247	47.860	34.160	20.625	1.00	26.30
ATOM	706	NE2	GLN	247	46.186	32.732	21.035	1.00	25.65
ATOM	707	C	GLN	247	51.098	33.374	24.528	1.00	22.10
ATOM	708	O							



ATOM	710	CA	ILE	248	51.379	35.042	26.276	1.00	23.21
ATOM	711	CB	ILE	248	50.473	35.824	27.273	1.00	24.59
ATOM	712	CG2	ILE	248	51.304	36.682	28.242	1.00	24.09
ATOM	713	CG1	ILE	248	49.499	36.707	26.487	1.00	23.47
ATOM	714	CD1	ILE	248	48.413	37.323	27.341	1.00	23.84
ATOM	715	C <sup>-</sup>	ILE	248	52.568	34.387	26.986	1.00	22.27
ATOM	716	O	ILE	248	53.705	34.833	26.829	1.00	22.06
ATOM	717	N	ILE	249	52.321	33.313	27.729	1.00	21.40
ATOM	718	CA	ILE	249	53.398	32.630	28.440	1.00	21.40
ATOM	719	CB	ILE	249	52.850	31.438	29.279	1.00	23.53
ATOM	720	CG2	ILE	249	53.972	30.489	29.711	1.00	21.44
ATOM	721	CG1	ILE	249	52.098	31.963	30.500	1.00	22.76
ATOM	722	CD1	ILE	249	51.252	30.911	31.175	1.00	25.03
ATOM	723	C	ILE	249	54.481	32.148	27.470	1.00	22.24
ATOM	724	O	ILE	249	55.677	32.321	27.733	1.00	22.90
ATOM	725	N	LEU	250	54.072	31.582	26.334	1.00	22.65
ATOM	726	CA	LEU	250	55.028	31.079	25.345	1.00	21.40
ATOM	727	CB	LEU	250	54.319	30.290	24.239	1.00	20.06
ATOM	728	CG	LEU	250	53.566	29.038	24.677	1.00	20.22
ATOM	729	CD1	LEU	250	52.952	28.406	23.453	1.00	19.19
ATOM	730	CD2	LEU	250	54.494	28.050	25.386	1.00	18.52
ATOM	731	C	LEU	250	55.850	32.209	24.736	1.00	20.82
ATOM	732	O	LEU	250	57.069	32.094	24.603	1.00	20.27
ATOM	733	N	LEU	251	55.179	33.302	24.384	1.00	22.14
ATOM	734	CA	LEU	251	55.842	34.467	23.805	1.00	22.90
ATOM	735	CB	LEU	251	54.806	35.543	23.471	1.00	22.76
ATOM	736	CG	LEU	251	54.513	35.899	22.012	1.00	23.35
ATOM	737	CD1	LEU	251	55.347	35.103	21.047	1.00	22.38
ATOM	738	CD2	LEU	251	53.040	35.708	21.747	1.00	22.86
ATOM	739	C	LEU	251	56.891	35.030	24.776	1.00	23.67
ATOM	740	O	LEU	251	58.051	35.234	24.402	1.00	22.58
ATOM	741	N	LYS	252	56.491	35.236	26.029	1.00	24.64
ATOM	742	CA	LYS	252	57.395	35.754	27.057	1.00	26.22
ATOM	743	CB	LYS	252	56.617	36.037	28.350	1.00	27.79
ATOM	744	CG	LYS	252	55.351	36.838	28.093	1.00	32.69
ATOM	745	CD	LYS	252	55.185	38.023	29.003	1.00	35.85
ATOM	746	CE	LYS	252	54.773	37.626	30.397	1.00	39.34
ATOM	747	NZ	LYS	252	54.477	38.870	31.168	1.00	44.60
ATOM	748	C	LYS	252	58.566	34.793	27.312	1.00	25.26
ATOM	749	O	LYS	252	59.701	35.222	27.555	1.00	26.67
ATOM	750	N	GLY	253	58.306	33.497	27.195	1.00	23.97
ATOM	751	CA	GLY	253	59.356	32.521	27.404	1.00	22.00
ATOM	752	C	GLY	253	60.397	32.429	26.292	1.00	23.10
ATOM	753	O	GLY	253	61.568	32.165	26.585	1.00	25.12
ATOM	754	N	CYS	254	60.014	32.702	25.041	1.00	22.27
ATOM	755								

ATOM	757	SG	CYS	254	58.992	32.385	21.893	1.00	22.92
ATOM	758	C	CYS	254	61.354	33.869	23.201	1.00	19.77
ATOM	759	O	CYS	254	62.215	33.834	22.316	1.00	19.88
ATOM	760	N	CYS	255	60.731	34.984	23.561	1.00	19.56
ATOM	761	CA	CYS	255	61.018	36.264	22.917	1.00	21.16
ATOM	762	CB	CYS	255	60.292	37.407	23.634	1.00	21.21
ATOM	763	SG	CYS	255	60.404	38.957	22.735	1.00	22.22
ATOM	764	C	CYS	255	62.504	36.590	22.775	1.00	21.36
ATOM	765	O	CYS	255	62.986	36.847	21.667	1.00	20.58
ATOM	766	N	MET	256	63.232	36.574	23.887	1.00	20.52
ATOM	767	CA	MET	256	64.657	36.874	23.835	1.00	20.07
ATOM	768	CB	MET	256	65.255	36.967	25.253	1.00	20.39
ATOM	769	CG	MET	256	66.744	37.360	25.267	1.00	19.20
ATOM	770	SD	MET	256	67.066	38.952	24.447	1.00	20.26
ATOM	771	CE	MET	256	68.856	38.971	24.375	1.00	18.47
ATOM	772	C	MET	256	65.408	35.830	23.005	1.00	18.75
ATOM	773	O	MET	256	66.305	36.164	22.225	1.00	18.15
ATOM	774	N	GLU	257	65.035	34.568	23.170	1.00	19.00
ATOM	775	CA	GLU	257	65.685	33.480	22.443	1.00	19.71
ATOM	776	CB	GLU	257	65.104	32.145	22.882	1.00	21.15
ATOM	777	CG	GLU	257	65.451	31.821	24.319	1.00	26.39
ATOM	778	CD	GLU	257	64.513	30.820	24.929	1.00	30.75
ATOM	779	OE1	GLU	257	63.875	30.069	24.162	1.00	32.36
ATOM	780	OE2	GLU	257	64.415	30.783	26.172	1.00	33.70
ATOM	781	C	GLU	257	65.545	33.648	20.940	1.00	18.54
ATOM	782	O	GLU	257	66.521	33.506	20.197	1.00	17.58
ATOM	783	N	ILE	258	64.336	33.977	20.497	1.00	17.78
ATOM	784	CA	ILE	258	64.101	34.176	19.081	1.00	17.60
ATOM	785	CB	ILE	258	62.590	34.267	18.765	1.00	16.35
ATOM	786	CG2	ILE	258	62.376	34.777	17.326	1.00	16.20
ATOM	787	CG1	ILE	258	61.935	32.884	18.980	1.00	17.24
ATOM	788	CD1	ILE	258	60.437	32.787	18.593	1.00	14.08
ATOM	789	C	ILE	258	64.872	35.408	18.595	1.00	19.11
ATOM	790	O	ILE	258	65.609	35.326	17.601	1.00	19.02
ATOM	791	N	MET	259	64.785	36.517	19.341	1.00	19.71
ATOM	792	CA	MET	259	65.486	37.744	18.956	1.00	18.43
ATOM	793	CB	MET	259	65.162	38.890	19.910	1.00	19.99
ATOM	794	CG	MET	259	63.700	39.278	19.962	1.00	21.15
ATOM	795	SD	MET	259	63.452	40.921	20.700	1.00	24.33
ATOM	796	CE	MET	259	63.769	40.595	22.415	1.00	22.50
ATOM	797	C	MET	259	66.993	37.540	18.888	1.00	18.64
ATOM	798	O	MET	259	67.638	37.993	17.941	1.00	19.96
ATOM	799	N	SER	260	67.556	36.858	19.884	1.00	17.37
ATOM	800	CA	SER	260	68.993	36.592	19.915	1.00	16.76
ATOM	801	CB	SER	260	69.387	35.840	21.195	1.00	17.25
ATOM	802	OG	SER	260	69.078				

ATOM	804	O	SER	260	70.460	35.941	18.137	1.00	16.62
ATOM	805	N	LEU	261	68.539	34.781	18.385	1.00	15.15
ATOM	806	CA	LEU	261	68.802	33.900	17.262	1.00	15.31
ATOM	807	CB	LEU	261	67.708	32.834	17.153	1.00	15.43
ATOM	808	CG	LEU	261	67.652	32.014	15.858	1.00	15.82
ATOM	809	CD1	LEU	261	68.963	31.251	15.621	1.00	16.35
ATOM	810	CD2	LEU	261	66.470	31.060	15.937	1.00	13.72
ATOM	811	C	LEU	261	68.839	34.741	16.001	1.00	16.31
ATOM	812	O	LEU	261	69.766	34.619	15.194	1.00	16.68
ATOM	813	N	ARG	262	67.848	35.620	15.853	1.00	16.47
ATOM	814	CA	ARG	262	67.778	36.493	14.680	1.00	16.66
ATOM	815	CB	ARG	262	66.475	37.279	14.693	1.00	16.00
ATOM	816	CG	ARG	262	65.291	36.404	14.354	1.00	15.62
ATOM	817	CD	ARG	262	63.995	37.167	14.378	1.00	17.31
ATOM	818	NE	ARG	262	62.967	36.454	13.628	1.00	20.09
ATOM	819	CZ	ARG	262	61.755	36.932	13.361	1.00	21.06
ATOM	820	NH1	ARG	262	61.390	38.136	13.787	1.00	19.02
ATOM	821	NH2	ARG	262	60.909	36.207	12.640	1.00	22.63
ATOM	822	C	ARG	262	69.003	37.396	14.527	1.00	16.80
ATOM	823	O	ARG	262	69.440	37.664	13.412	1.00	16.82
ATOM	824	N	ALA	263	69.578	37.832	15.650	1.00	17.77
ATOM	825	CA	ALA	263	70.795	38.647	15.637	1.00	18.41
ATOM	826	CB	ALA	263	70.996	39.337	17.004	1.00	18.26
ATOM	827	C	ALA	263	71.998	37.740	15.327	1.00	19.15
ATOM	828	O	ALA	263	72.837	38.063	14.475	1.00	19.40
ATOM	829	N	ALA	264	72.056	36.587	15.996	1.00	19.84
ATOM	830	CA	ALA	264	73.155	35.633	15.818	1.00	20.35
ATOM	831	CB	ALA	264	73.045	34.483	16.832	1.00	18.09
ATOM	832	C	ALA	264	73.289	35.079	14.398	1.00	20.66
ATOM	833	O	ALA	264	74.406	34.870	13.922	1.00	21.04
ATOM	834	N	VAL	265	72.173	34.822	13.723	1.00	21.14
ATOM	835	CA	VAL	265	72.249	34.299	12.358	1.00	22.96
ATOM	836	CB	VAL	265	70.910	33.660	11.879	1.00	21.04
ATOM	837	CG1	VAL	265	70.458	32.600	12.866	1.00	19.48
ATOM	838	CG2	VAL	265	69.838	34.708	11.698	1.00	18.96
ATOM	839	C	VAL	265	72.718	35.387	11.382	1.00	24.66
ATOM	840	O	VAL	265	73.026	35.103	10.224	1.00	26.03
ATOM	841	N	ARG	266	72.777	36.628	11.858	1.00	25.11
ATOM	842	CA	ARG	266	73.233	37.729	11.031	1.00	25.60
ATOM	843	CB	ARG	266	72.187	38.819	10.964	1.00	24.09
ATOM	844	CG	ARG	266	71.035	38.427	10.088	1.00	23.37
ATOM	845	CD	ARG	266	69.998	39.492	10.098	1.00	24.80
ATOM	846	NE	ARG	266	68.961	39.253	9.109	1.00	24.01
ATOM	847	CZ	ARG	266	67.833	39.940	9.069	1.00	23.26
ATOM	848	NH1	ARG	266	67.613	40.880	9.970	1.00	24.16
ATOM	849	NH2	ARG	266	66.960	39.733	8.099	1.00	23.31
ATOM	850	C	ARG	266	74.543	38.273	11.543	1.00	28.07

ATOM	851	O	ARG	266	74.786	39.479	11.517	1.00	29.67
ATOM	852	N	TYR	267	75.367	37.366	12.053	1.00	28.90
ATOM	853	CA	TYR	267	76.679	37.714	12.558	1.00	30.23
ATOM	854	CB	TYR	267	77.223	36.584	13.434	1.00	29.98
ATOM	855	CG	TYR	267	78.699	36.702	13.727	1.00	31.75
ATOM	856	CD1	TYR	267	79.179	37.577	14.712	1.00	31.21
ATOM	857	CE1	TYR	267	80.544	37.705	14.950	1.00	31.29
ATOM	858	CD2	TYR	267	79.625	35.958	12.994	1.00	31.84
ATOM	859	CE2	TYR	267	80.986	36.078	13.222	1.00	32.15
ATOM	860	CZ	TYR	267	81.442	36.949	14.197	1.00	32.60
ATOM	861	OH	TYR	267	82.801	37.052	14.389	1.00	34.13
ATOM	862	C	TYR	267	77.570	37.900	11.343	1.00	31.17
ATOM	863	O	TYR	267	77.543	37.086	10.426	1.00	30.91
ATOM	864	N	ASP	268	78.361	38.966	11.336	1.00	33.09
ATOM	865	CA	ASP	268	79.252	39.233	10.216	1.00	35.57
ATOM	866	CB	ASP	268	79.085	40.679	9.747	1.00	39.39
ATOM	867	CG	ASP	268	79.796	40.954	8.432	1.00	42.22
ATOM	868	OD1	ASP	268	79.426	40.331	7.412	1.00	46.07
ATOM	869	OD2	ASP	268	80.718	41.798	8.415	1.00	44.30
ATOM	870	C	ASP	268	80.700	38.967	10.620	1.00	35.72
ATOM	871	O	ASP	268	81.287	39.737	11.384	1.00	34.49
ATOM	872	N	PRO	269	81.295	37.872	10.108	1.00	37.00
ATOM	873	CD	PRO	269	80.712	36.887	9.182	1.00	36.77
ATOM	874	CA	PRO	269	82.679	37.514	10.427	1.00	38.52
ATOM	875	CB	PRO	269	82.905	36.239	9.611	1.00	37.06
ATOM	876	CG	PRO	269	81.549	35.669	9.453	1.00	36.19
ATOM	877	C	PRO	269	83.656	38.613	10.019	1.00	40.96
ATOM	878	O	PRO	269	84.586	38.929	10.760	1.00	42.23
ATOM	879	N	ALA	270	83.418	39.209	8.854	1.00	41.92
ATOM	880	CA	ALA	270	84.277	40.272	8.342	1.00	42.08
ATOM	881	CB	ALA	270	83.709	40.838	7.029	1.00	42.64
ATOM	882	C	ALA	270	84.495	41.394	9.355	1.00	41.70
ATOM	883	O	ALA	270	85.632	41.709	9.684	1.00	42.25
ATOM	884	N	SER	271	83.408	41.970	9.865	1.00	41.87
ATOM	885	CA	SER	271	83.495	43.073	10.830	1.00	40.75
ATOM	886	CB	SER	271	82.454	44.143	10.500	1.00	40.60
ATOM	887	OG	SER	271	81.150	43.590	10.464	1.00	40.31
ATOM	888	C	SER	271	83.344	42.658	12.290	1.00	39.99
ATOM	889	O	SER	271	83.484	43.487	13.194	1.00	38.77
ATOM	890	N	ASP	272	83.042	41.381	12.508	1.00	38.94
ATOM	891	CA	ASP	272	82.859	40.844	13.845	1.00	37.78
ATOM	892	CB	ASP	272	84.182	40.904	14.625	1.00	38.86
ATOM	893	CG	ASP	272	84.094	40.255	16.000	1.00	41.09
ATOM	894	OD1	ASP	272	83.342	39.275	16.173	1.00	41.64
ATOM	895	OD2	ASP	272	84.781	40.734	16.924	1.00	43.84
ATOM	896	C	ASP	272	81.744	41.634			



ATOM	898	N	THR	273	80.603	41.723	13.865	1.00	33.65
ATOM	899	CA	THR	273	79.469	42.443	14.425	1.00	31.57
ATOM	900	CB	THR	273	79.246	43.790	13.695	1.00	31.69
ATOM	901	OG1	THR	273	79.087	43.557	12.289	1.00	30.71
ATOM	902	CG2	THR	273	80.426	44.730	13.922	1.00	31.53
ATOM	903	C	THR	273	78.184	41.631	14.310	1.00	30.15
ATOM	904	O	THR	273	78.104	40.697	13.504	1.00	30.10
ATOM	905	N	LEU	274	77.213	41.942	15.164	1.00	27.09
ATOM	906	CA	LEU	274	75.907	41.303	15.103	1.00	25.94
ATOM	907	CB	LEU	274	75.396	40.936	16.496	1.00	24.47
ATOM	908	CG	LEU	274	76.020	39.731	17.206	1.00	23.33
ATOM	909	CD1	LEU	274	75.436	39.631	18.602	1.00	21.14
ATOM	910	CD2	LEU	274	75.792	38.444	16.427	1.00	20.04
ATOM	911	C	LEU	274	75.010	42.377	14.500	1.00	26.57
ATOM	912	O	LEU	274	75.339	43.557	14.568	1.00	27.03
ATOM	913	N	THR	275	73.914	41.987	13.865	1.00	26.60
ATOM	914	CA	THR	275	73.009	42.966	13.285	1.00	26.48
ATOM	915	CB	THR	275	72.786	42.717	11.781	1.00	26.52
ATOM	916	OG1	THR	275	74.044	42.719	11.097	1.00	28.67
ATOM	917	CG2	THR	275	71.919	43.799	11.198	1.00	27.35
ATOM	918	C	THR	275	71.674	42.898	14.014	1.00	26.57
ATOM	919	O	THR	275	71.069	41.825	14.121	1.00	28.50
ATOM	920	N	LEU	276	71.236	44.026	14.564	1.00	25.18
ATOM	921	CA	LEU	276	69.970	44.069	15.276	1.00	24.61
ATOM	922	CB	LEU	276	70.057	44.987	16.506	1.00	23.61
ATOM	923	CG	LEU	276	71.199	44.730	17.503	1.00	24.36
ATOM	924	CD1	LEU	276	71.039	45.654	18.709	1.00	19.91
ATOM	925	CD2	LEU	276	71.225	43.253	17.947	1.00	22.20
ATOM	926	C	LEU	276	68.894	44.560	14.322	1.00	25.63
ATOM	927	O	LEU	276	69.100	45.556	13.623	1.00	25.35
ATOM	928	N	SER	277	67.787	43.814	14.249	1.00	25.94
ATOM	929	CA	SER	277	66.634	44.141	13.403	1.00	24.61
ATOM	930	CB	SER	277	65.874	45.335	13.987	1.00	21.96
ATOM	931	OG	SER	277	65.368	45.029	15.273	1.00	19.68
ATOM	932	C	SER	277	67.005	44.406	11.946	1.00	25.20
ATOM	933	O	SER	277	66.350	45.199	11.267	1.00	25.21
ATOM	934	N	GLY	278	68.067	43.747	11.489	1.00	27.08
ATOM	935	CA	GLY	278	68.556	43.899	10.127	1.00	29.27
ATOM	936	C	GLY	278	69.022	45.297	9.753	1.00	31.57
ATOM	937	O	GLY	278	69.303	45.564	8.591	1.00	31.42
ATOM	938	N	GLU	279	69.159	46.177	10.740	1.00	33.41
ATOM	939	CA	GLU	279	69.558	47.560	10.484	1.00	34.84
ATOM	940	CB	GLU	279	68.345	48.485	10.650	1.00	36.16
ATOM	941	CG	GLU	279	67.843	48.606	12.090	1.00	38.08
ATOM	942	CD	GLU	279	66.566	49.419	12.206	1.00	41.07
ATOM	943	OE1	GLU						



ATOM	945	C	GLU	279	70.706	48.116	11.326	1.00	34.38
ATOM	946	O	GLU	279	71.366	49.057	10.901	1.00	35.60
ATOM	947	N	MET	280	70.944	47.565	12.511	1.00	33.43
ATOM	948	CA	MET	280	72.014	48.085	13.358	1.00	32.27
ATOM	949	CB	MET	280	71.443	48.544	14.702	1.00	31.81
ATOM	950	CG	MET	280	72.471	49.181	15.637	1.00	29.76
ATOM	951	SD	MET	280	71.813	49.482	17.289	1.00	29.63
ATOM	952	CE	MET	280	70.592	50.735	16.989	1.00	24.91
ATOM	953	C	MET	280	73.161	47.119	13.603	1.00	32.51
ATOM	954	O	MET	280	72.995	46.117	14.303	1.00	32.78
ATOM	955	N	ALA	281	74.321	47.408	13.021	1.00	31.74
ATOM	956	CA	ALA	281	75.491	46.564	13.231	1.00	32.25
ATOM	957	CB	ALA	281	76.494	46.740	12.108	1.00	30.91
ATOM	958	C	ALA	281	76.091	47.006	14.563	1.00	33.09
ATOM	959	O	ALA	281	76.261	48.202	14.805	1.00	34.06
ATOM	960	N	VAL	282	76.358	46.053	15.447	1.00	33.78
ATOM	961	CA	VAL	282	76.913	46.366	16.755	1.00	33.45
ATOM	962	CB	VAL	282	75.858	46.208	17.885	1.00	34.92
ATOM	963	CG1	VAL	282	74.775	47.269	17.744	1.00	34.90
ATOM	964	CG2	VAL	282	75.246	44.806	17.860	1.00	34.39
ATOM	965	C	VAL	282	78.119	45.514	17.087	1.00	33.93
ATOM	966	O	VAL	282	78.202	44.347	16.702	1.00	35.11
ATOM	967	N	LYS	283	79.071	46.123	17.777	1.00	33.49
ATOM	968	CA	LYS	283	80.285	45.446	18.187	1.00	34.83
ATOM	969	CB	LYS	283	81.446	46.445	18.183	1.00	35.96
ATOM	970	CG	LYS	283	81.726	47.013	16.797	1.00	39.20
ATOM	971	CD	LYS	283	82.621	48.245	16.844	1.00	43.38
ATOM	972	CE	LYS	283	83.142	48.611	15.455	1.00	44.17
ATOM	973	NZ	LYS	283	84.077	47.563	14.922	1.00	47.27
ATOM	974	C	LYS	283	80.068	44.832	19.572	1.00	33.94
ATOM	975	O	LYS	283	79.134	45.215	20.290	1.00	33.85
ATOM	976	N	ARG	284	80.939	43.895	19.941	1.00	33.63
ATOM	977	CA	ARG	284	80.873	43.184	21.217	1.00	34.00
ATOM	978	CB	ARG	284	82.094	42.285	21.381	1.00	34.04
ATOM	979	CG	ARG	284	82.332	41.369	20.219	1.00	36.31
ATOM	980	CD	ARG	284	83.638	40.643	20.354	1.00	37.03
ATOM	981	NE	ARG	284	83.724	39.576	19.369	1.00	39.27
ATOM	982	CZ	ARG	284	83.323	38.326	19.583	1.00	40.07
ATOM	983	NH1	ARG	284	82.804	37.973	20.759	1.00	39.78
ATOM	984	NH2	ARG	284	83.434	37.428	18.613	1.00	40.16
ATOM	985	C	ARG	284	80.787	44.101	22.419	1.00	35.16
ATOM	986	O	ARG	284	79.884	43.977	23.249	1.00	35.87
ATOM	987	N	GLU	285	81.763	44.993	22.530	1.00	35.75
ATOM	988	CA	GLU	285	81.827	45.939	23.632	1.00	36.86
ATOM	989	CB	GLU	285	83.071	46.818	23.464	1.00	40.47
ATOM	990	CG	GLU	285	83.20				

ATOM	992	OE1	GLU	285	84.784	49.657	23.760	1.00	55.37
ATOM	993	OE2	GLU	285	82.686	49.942	23.176	1.00	56.95
ATOM	994	C	GLU	285	80.552	46.785	23.684	1.00	34.45
ATOM	995	O	GLU	285	79.990	47.007	24.754	1.00	34.47
ATOM	996	N	GLN	286	80.046	47.166	22.515	1.00	32.27
ATOM	997	CA	GLN	286	78.853	47.991	22.438	1.00	30.35
ATOM	998	CB	GLN	286	78.615	48.472	21.006	1.00	33.34
ATOM	999	CG	GLN	286	79.632	49.497	20.500	1.00	35.09
ATOM	1000	CD	GLN	286	79.293	50.023	19.108	1.00	38.42
ATOM	1001	OE1	GLN	286	79.161	49.248	18.158	1.00	39.03
ATOM	1002	NE2	GLN	286	79.156	51.339	18.982	1.00	37.82
ATOM	1003	C	GLN	286	77.605	47.308	22.970	1.00	29.57
ATOM	1004	O	GLN	286	76.870	47.891	23.770	1.00	26.96
ATOM	1005	N	LEU	287	77.352	46.080	22.524	1.00	29.50
ATOM	1006	CA	LEU	287	76.164	45.350	22.979	1.00	28.93
ATOM	1007	CB	LEU	287	75.831	44.182	22.029	1.00	27.14
ATOM	1008	CG	LEU	287	74.474	43.484	22.227	1.00	24.66
ATOM	1009	CD1	LEU	287	73.316	44.475	22.184	1.00	22.70
ATOM	1010	CD2	LEU	287	74.297	42.413	21.163	1.00	25.17
ATOM	1011	C	LEU	287	76.303	44.874	24.433	1.00	28.10
ATOM	1012	O	LEU	287	75.301	44.748	25.155	1.00	28.58
ATOM	1013	N	LYS	288	77.541	44.652	24.868	1.00	27.97
ATOM	1014	CA	LYS	288	77.808	44.218	26.230	1.00	28.55
ATOM	1015	CB	LYS	288	79.270	43.800	26.376	1.00	28.93
ATOM	1016	CG	LYS	288	79.603	43.254	27.750	1.00	32.46
ATOM	1017	CD	LYS	288	81.015	42.725	27.826	1.00	33.48
ATOM	1018	CE	LYS	288	81.205	41.878	29.071	1.00	35.76
ATOM	1019	NZ	LYS	288	82.525	41.186	29.029	1.00	40.52
ATOM	1020	C	LYS	288	77.497	45.341	27.220	1.00	29.15
ATOM	1021	O	LYS	288	76.782	45.132	28.207	1.00	31.28
ATOM	1022	N	ASN	289	77.996	46.539	26.933	1.00	28.58
ATOM	1023	CA	ASN	289	77.794	47.692	27.811	1.00	28.40
ATOM	1024	CB	ASN	289	78.815	48.775	27.485	1.00	28.28
ATOM	1025	CG	ASN	289	80.224	48.329	27.770	1.00	31.30
ATOM	1026	OD1	ASN	289	80.445	47.442	28.601	1.00	33.02
ATOM	1027	ND2	ASN	289	81.190	48.928	27.087	1.00	30.49
ATOM	1028	C	ASN	289	76.395	48.278	27.792	1.00	28.33
ATOM	1029	O	ASN	289	76.005	48.977	28.724	1.00	28.36
ATOM	1030	N	GLY	290	75.638	47.977	26.740	1.00	26.71
ATOM	1031	CA	GLY	290	74.286	48.487	26.606	1.00	23.27
ATOM	1032	C	GLY	290	73.233	47.852	27.484	1.00	22.93
ATOM	1033	O	GLY	290	72.063	48.219	27.399	1.00	23.84
ATOM	1034	N	GLY	291	73.620	46.905	28.330	1.00	21.30
ATOM	1035	CA	GLY	291	72.637	46.290	29.199	1.00	20.38
ATOM	1036	C	GLY	291	72.653	44.778	29.200		

ATOM	1039	CA	LEU	292	73.248	42.717	28.062	1.00	21.51
ATOM	1040	CB	LEU	292	73.319	42.280	26.593	1.00	18.52
ATOM	1041	CG	LEU	292	72.019	42.506	25.815	1.00	17.07
ATOM	1042	CD1	LEU	292	72.103	41.818	24.479	1.00	18.09
ATOM	1043	CD2	LEU	292	70.844	41.947	26.599	1.00	16.35
ATOM	1044	C	LEU	292	74.347	42.046	28.872	1.00	22.17
ATOM	1045	O	LEU	292	74.176	40.923	29.352	1.00	21.91
ATOM	1046	N	GLY	293	75.479	42.724	29.011	1.00	23.76
ATOM	1047	CA	GLY	293	76.588	42.169	29.760	1.00	23.92
ATOM	1048	C	GLY	293	77.134	40.926	29.091	1.00	25.09
ATOM	1049	O	GLY	293	77.362	40.919	27.883	1.00	26.51
ATOM	1050	N	VAL	294	77.332	39.866	29.867	1.00	26.08
ATOM	1051	CA	VAL	294	77.854	38.618	29.329	1.00	26.34
ATOM	1052	CB	VAL	294	78.263	37.636	30.443	1.00	26.97
ATOM	1053	CG1	VAL	294	79.440	38.199	31.209	1.00	28.20
ATOM	1054	CG2	VAL	294	77.099	37.371	31.384	1.00	25.56
ATOM	1055	C	VAL	294	76.891	37.937	28.360	1.00	26.41
ATOM	1056	O	VAL	294	77.315	37.097	27.568	1.00	27.65
ATOM	1057	N	VAL	295	75.608	38.304	28.408	1.00	26.09
ATOM	1058	CA	VAL	295	74.606	37.740	27.499	1.00	26.65
ATOM	1059	CB	VAL	295	73.186	38.312	27.777	1.00	28.39
ATOM	1060	CG1	VAL	295	72.164	37.740	26.782	1.00	26.69
ATOM	1061	CG2	VAL	295	72.763	38.005	29.206	1.00	26.23
ATOM	1062	C	VAL	295	75.035	38.089	26.069	1.00	25.83
ATOM	1063	O	VAL	295	74.903	37.286	25.151	1.00	27.12
ATOM	1064	N	SER	296	75.609	39.275	25.908	1.00	24.95
ATOM	1065	CA	SER	296	76.097	39.725	24.619	1.00	26.17
ATOM	1066	CB	SER	296	76.665	41.132	24.742	1.00	25.82
ATOM	1067	OG	SER	296	77.253	41.554	23.525	1.00	26.64
ATOM	1068	C	SER	296	77.196	38.783	24.142	1.00	28.63
ATOM	1069	O	SER	296	77.241	38.420	22.963	1.00	29.19
ATOM	1070	N	ASP	297	78.118	38.443	25.046	1.00	29.69
ATOM	1071	CA	ASP	297	79.211	37.531	24.731	1.00	28.96
ATOM	1072	CB	ASP	297	80.058	37.234	25.973	1.00	31.82
ATOM	1073	CG	ASP	297	80.768	38.454	26.506	1.00	35.23
ATOM	1074	OD1	ASP	297	80.958	39.429	25.743	1.00	35.71
ATOM	1075	OD2	ASP	297	81.140	38.430	27.698	1.00	37.68
ATOM	1076	C	ASP	297	78.605	36.227	24.247	1.00	27.63
ATOM	1077	O	ASP	297	79.048	35.666	23.248	1.00	29.88
ATOM	1078	N	ALA	298	77.581	35.762	24.952	1.00	25.15
ATOM	1079	CA	ALA	298	76.909	34.527	24.592	1.00	24.49
ATOM	1080	CB	ALA	298	75.811	34.224	25.594	1.00	21.91
ATOM	1081	C	ALA	298	76.343	34.569	23.158	1.00	24.93
ATOM	1082	O	ALA	298	76.589	33.654	22.357	1.00	24.83
ATOM	1083	N	ILE	299	75.632	35.647	22.814	1.00	24.70

ATOM	1086	CG2 ILE	299	73.338	36.876	20.005	1.00	19.17
ATOM	1087	CG1 ILE	299	72.994	36.876	22.459	1.00	21.16
ATOM	1088	CD1 ILE	299	72.363	38.228	22.853	1.00	22.04
ATOM	1089	C ILE	299	76.127	35.829	20.428	1.00	22.33
ATOM	1090	O ILE	299	75.995	35.234	19.367	1.00	24.80
ATOM	1091	N PHE	300	77.209	36.538	20.724	1.00	21.92
ATOM	1092	CA PHE	300	78.322	36.641	19.785	1.00	23.08
ATOM	1093	CB PHE	300	79.385	37.636	20.278	1.00	24.08
ATOM	1094	CG PHE	300	79.249	39.017	19.686	1.00	24.18
ATOM	1095	CD1 PHE	300	78.494	39.991	20.325	1.00	22.64
ATOM	1096	CD2 PHE	300	79.857	39.331	18.471	1.00	23.76
ATOM	1097	CE1 PHE	300	78.347	41.253	19.770	1.00	22.38
ATOM	1098	CE2 PHE	300	79.715	40.596	17.904	1.00	23.21
ATOM	1099	CZ PHE	300	78.957	41.558	18.554	1.00	22.46
ATOM	1100	C PHE	300	78.948	35.274	19.561	1.00	23.06
ATOM	1101	O PHE	300	79.264	34.913	18.426	1.00	23.97
ATOM	1102	N GLU	301	79.113	34.506	20.636	1.00	23.75
ATOM	1103	CA GLU	301	79.694	33.169	20.525	1.00	24.16
ATOM	1104	CB GLU	301	79.884	32.545	21.902	1.00	23.03
ATOM	1105	C GLU	301	78.776	32.302	19.672	1.00	23.62
ATOM	1106	O GLU	301	79.240	31.591	18.777	1.00	25.11
ATOM	1107	N LEU	302	77.472	32.394	19.926	1.00	23.12
ATOM	1108	CA LEU	302	76.495	31.624	19.166	1.00	23.56
ATOM	1109	CB LEU	302	75.082	31.865	19.701	1.00	21.75
ATOM	1110	CG LEU	302	73.953	31.120	18.979	1.00	22.61
ATOM	1111	CD1 LEU	302	74.084	29.612	19.193	1.00	22.31
ATOM	1112	CD2 LEU	302	72.611	31.604	19.485	1.00	19.27
ATOM	1113	C LEU	302	76.588	32.011	17.687	1.00	24.41
ATOM	1114	O LEU	302	76.670	31.140	16.814	1.00	24.63
ATOM	1115	N GLY	303	76.651	33.316	17.425	1.00	25.69
ATOM	1116	CA GLY	303	76.746	33.816	16.062	1.00	25.87
ATOM	1117	C GLY	303	77.975	33.288	15.338	1.00	28.63
ATOM	1118	O GLY	303	77.893	32.895	14.170	1.00	28.30
ATOM	1119	N LYS	304	79.116	33.279	16.023	1.00	29.53
ATOM	1120	CA LYS	304	80.360	32.791	15.437	1.00	31.18
ATOM	1121	CB LYS	304	81.529	32.931	16.418	1.00	34.79
ATOM	1122	CG LYS	304	82.157	34.307	16.506	1.00	40.28
ATOM	1123	CD LYS	304	83.441	34.262	17.332	1.00	44.37
ATOM	1124	CE LYS	304	83.174	33.814	18.775	1.00	47.63
ATOM	1125	NZ LYS	304	82.459	34.847	19.592	1.00	48.83
ATOM	1126	C LYS	304	80.245	31.328	15.042	1.00	30.87
ATOM	1127	O LYS	304	80.632	30.944	13.932	1.00	29.53
ATOM	1128	N SER	305	79.720	30.518	15.961	1.00	30.46
ATOM	1129	CA SER	305	79.566	29.086	15.731	1.00	31.09
ATOM	1130	CB SER	305	79.243	28.370	17.041	1.00	29.83
ATOM	1131	OG SER	305	77.990	28.783	17.550	1.00	34.66
ATOM	1132	C SER	305	78.532	28.732	14.653	1.00	31.06



ATOM	1133	O	SER	305	78.745	27.799	13.872	1.00	31.84
ATOM	1134	N	LEU	306	77.436	29.491	14.594	1.00	29.43
ATOM	1135	CA	LEU	306	76.378	29.258	13.611	1.00	28.39
ATOM	1136	CB	LEU	306	75.121	30.055	13.962	1.00	26.05
ATOM	1137	CG	LEU	306	74.306	29.573	15.157	1.00	26.33
ATOM	1138	CD1	LEU	306	73.061	30.430	15.285	1.00	26.22
ATOM	1139	CD2	LEU	306	73.924	28.110	14.985	1.00	25.86
ATOM	1140	C	LEU	306	76.754	29.529	12.157	1.00	28.66
ATOM	1141	O	LEU	306	76.116	29.001	11.253	1.00	28.58
ATOM	1142	N	SER	307	77.786	30.338	11.931	1.00	29.72
ATOM	1143	CA	SER	307	78.224	30.667	10.577	1.00	31.19
ATOM	1144	CB	SER	307	79.466	31.556	10.617	1.00	30.15
ATOM	1145	OG	SER	307	79.226	32.710	11.396	1.00	35.19
ATOM	1146	C	SER	307	78.531	29.412	9.777	1.00	32.75
ATOM	1147	O	SER	307	78.110	29.283	8.621	1.00	33.09
ATOM	1148	N	ALA	308	79.248	28.482	10.407	1.00	33.36
ATOM	1149	CA	ALA	308	79.626	27.223	9.769	1.00	34.50
ATOM	1150	CB	ALA	308	80.636	26.473	10.637	1.00	33.55
ATOM	1151	C	ALA	308	78.417	26.328	9.466	1.00	35.00
ATOM	1152	O	ALA	308	78.469	25.501	8.550	1.00	37.10
ATOM	1153	N	PHE	309	77.335	26.496	10.226	1.00	32.76
ATOM	1154	CA	PHE	309	76.134	25.698	10.028	1.00	31.73
ATOM	1155	CB	PHE	309	75.214	25.818	11.232	1.00	30.04
ATOM	1156	CG	PHE	309	75.705	25.091	12.438	1.00	31.19
ATOM	1157	CD1	PHE	309	74.973	24.048	12.975	1.00	31.61
ATOM	1158	CD2	PHE	309	76.884	25.459	13.054	1.00	31.92
ATOM	1159	CE1	PHE	309	75.400	23.391	14.110	1.00	31.22
ATOM	1160	CE2	PHE	309	77.320	24.807	14.194	1.00	31.01
ATOM	1161	CZ	PHE	309	76.577	23.771	14.720	1.00	30.47
ATOM	1162	C	PHE	309	75.364	26.050	8.753	1.00	31.53
ATOM	1163	O	PHE	309	74.516	25.269	8.310	1.00	31.28
ATOM	1164	N	ASN	310	75.661	27.220	8.181	1.00	31.12
ATOM	1165	CA	ASN	310	75.020	27.711	6.957	1.00	30.34
ATOM	1166	CB	ASN	310	75.636	27.036	5.719	1.00	31.63
ATOM	1167	C	ASN	310	73.511	27.492	7.003	1.00	29.40
ATOM	1168	O	ASN	310	72.939	26.791	6.156	1.00	29.15
ATOM	1169	N	LEU	311	72.875	28.055	8.026	1.00	27.60
ATOM	1170	CA	LEU	311	71.435	27.907	8.205	1.00	28.23
ATOM	1171	CB	LEU	311	71.021	28.313	9.621	1.00	27.41
ATOM	1172	CG	LEU	311	71.603	27.558	10.822	1.00	26.80
ATOM	1173	CD1	LEU	311	70.949	28.078	12.112	1.00	25.05
ATOM	1174	CD2	LEU	311	71.360	26.062	10.662	1.00	24.72
ATOM	1175	C	LEU	311	70.628	28.719	7.192	1.00	29.01
ATOM	1176	O	LEU	311	71.040	29.808	6.782	1.00	30.66
ATOM	1177	N	ASP	312	69.503	28.168	6.748	1.00	26.30
ATOM	117								



ATOM	1180	CG ASP	312	67.438	26.890	4.754	1.00	21.34
ATOM	1181	OD1 ASP	312	66.959	26.631	5.868	1.00	22.47
ATOM	1182	OD2 ASP	312	67.154	26.206	3.758	1.00	22.18
ATOM	1183	C ASP	312	67.419	29.379	6.542	1.00	24.49
ATOM	1184	O ASP	312	67.221	29.056	7.725	1.00	24.01
ATOM	1185	N <sup>+</sup> ASP	313	66.587	30.153	5.845	1.00	23.40
ATOM	1186	CA ASP	313	65.363	30.697	6.421	1.00	22.63
ATOM	1187	CB ASP	313	64.557	31.486	5.385	1.00	24.99
ATOM	1188	CG ASP	313	65.224	32.799	4.994	1.00	28.02
ATOM	1189	OD1 ASP	313	66.036	33.334	5.778	1.00	30.34
ATOM	1190	OD2 ASP	313	64.936	33.306	3.897	1.00	30.41
ATOM	1191	C ASP	313	64.480	29.650	7.053	1.00	21.47
ATOM	1192	O ASP	313	63.853	29.917	8.082	1.00	21.76
ATOM	1193	N THR	314	64.407	28.474	6.435	1.00	19.16
ATOM	1194	CA THR	314	63.580	27.386	6.966	1.00	18.79
ATOM	1195	CB THR	314	63.398	26.240	5.913	1.00	19.68
ATOM	1196	OG1 THR	314	62.743	26.758	4.747	1.00	20.56
ATOM	1197	CG2 THR	314	62.558	25.112	6.482	1.00	18.84
ATOM	1198	C THR	314	64.133	26.818	8.293	1.00	15.38
ATOM	1199	O THR	314	63.383	26.538	9.223	1.00	14.08
ATOM	1200	N GLU	315	65.445	26.656	8.376	1.00	15.16
ATOM	1201	CA GLU	315	66.051	26.126	9.593	1.00	16.78
ATOM	1202	CB GLU	315	67.513	25.785	9.340	1.00	14.29
ATOM	1203	CG GLU	315	67.611	24.483	8.579	1.00	15.13
ATOM	1204	CD GLU	315	68.910	24.291	7.872	1.00	15.90
ATOM	1205	OE1 GLU	315	69.625	25.285	7.639	1.00	19.80
ATOM	1206	OE2 GLU	315	69.211	23.129	7.527	1.00	19.34
ATOM	1207	C GLU	315	65.872	27.119	10.736	1.00	17.27
ATOM	1208	O GLU	315	65.457	26.742	11.836	1.00	17.46
ATOM	1209	N VAL	316	66.081	28.399	10.440	1.00	17.12
ATOM	1210	CA VAL	316	65.897	29.441	11.446	1.00	16.92
ATOM	1211	CB VAL	316	66.336	30.828	10.918	1.00	15.89
ATOM	1212	CG1 VAL	316	66.062	31.921	11.962	1.00	14.60
ATOM	1213	CG2 VAL	316	67.811	30.785	10.579	1.00	15.95
ATOM	1214	C VAL	316	64.430	29.472	11.869	1.00	17.32
ATOM	1215	O VAL	316	64.131	29.582	13.055	1.00	18.11
ATOM	1216	N ALA	317	63.515	29.324	10.905	1.00	17.42
ATOM	1217	CA ALA	317	62.076	29.342	11.195	1.00	16.21
ATOM	1218	CB ALA	317	61.262	29.321	9.910	1.00	14.63
ATOM	1219	C ALA	317	61.656	28.181	12.079	1.00	16.84
ATOM	1220	O ALA	317	60.904	28.359	13.036	1.00	16.08
ATOM	1221	N LEU	318	62.146	26.990	11.759	1.00	17.27
ATOM	1222	CA LEU	318	61.783	25.804	12.526	1.00	17.88
ATOM	1223	CB LEU	318	62.141	24.525	11.748	1.00	17.58
ATOM	1224	CG LEU	318	61.331	24.333	10.439	1.00	16.87
ATOM	1225	CD1 LEU	318	61.837	23.155	9.658	1.00	15.79
ATOM	1226	CD2 LEU	318	59.860	24.149	10.728	1.00	14.08

ATOM	1227	C	LEU	318	62.394	25.852	13.932	1.00	18.20
ATOM	1228	O	LEU	318	61.733	25.495	14.910	1.00	18.71
ATOM	1229	N	LEU	319	63.614	26.380	14.034	1.00	17.73
ATOM	1230	CA	LEU	319	64.288	26.531	15.321	1.00	16.57
ATOM	1231	CB	LEU	319	65.689	27.105	15.107	1.00	18.81
ATOM	1232	CG	LEU	319	66.733	27.223	16.224	1.00	21.77
ATOM	1233	CD1	LEU	319	66.767	25.994	17.117	1.00	23.03
ATOM	1234	CD2	LEU	319	68.076	27.421	15.554	1.00	20.86
ATOM	1235	C	LEU	319	63.433	27.471	16.160	1.00	16.07
ATOM	1236	O	LEU	319	63.134	27.183	17.319	1.00	16.40
ATOM	1237	N	GLN	320	62.948	28.546	15.545	1.00	13.91
ATOM	1238	CA	GLN	320	62.101	29.490	16.253	1.00	13.86
ATOM	1239	CB	GLN	320	61.782	30.697	15.373	1.00	13.26
ATOM	1240	CG	GLN	320	62.994	31.553	15.080	1.00	12.17
ATOM	1241	CD	GLN	320	62.691	32.802	14.253	1.00	13.98
ATOM	1242	OE1	GLN	320	63.597	33.568	13.950	1.00	15.61
ATOM	1243	NE2	GLN	320	61.436	32.993	13.862	1.00	13.85
ATOM	1244	C	GLN	320	60.813	28.832	16.746	1.00	14.52
ATOM	1245	O	GLN	320	60.367	29.087	17.864	1.00	15.12
ATOM	1246	N	ALA	321	60.211	27.982	15.924	1.00	14.21
ATOM	1247	CA	ALA	321	58.976	27.298	16.309	1.00	15.04
ATOM	1248	CB	ALA	321	58.408	26.519	15.115	1.00	13.84
ATOM	1249	C	ALA	321	59.217	26.349	17.487	1.00	15.98
ATOM	1250	O	ALA	321	58.358	26.197	18.355	1.00	15.12
ATOM	1251	N	VAL	322	60.373	25.687	17.488	1.00	16.63
ATOM	1252	CA	VAL	322	60.720	24.757	18.557	1.00	18.74
ATOM	1253	CB	VAL	322	62.012	23.943	18.231	1.00	19.42
ATOM	1254	CG1	VAL	322	62.493	23.154	19.455	1.00	19.45
ATOM	1255	CG2	VAL	322	61.745	22.986	17.083	1.00	19.05
ATOM	1256	C	VAL	322	60.910	25.556	19.833	1.00	18.42
ATOM	1257	O	VAL	322	60.421	25.164	20.886	1.00	19.46
ATOM	1258	N	LEU	323	61.607	26.685	19.735	1.00	18.65
ATOM	1259	CA	LEU	323	61.836	27.543	20.894	1.00	18.49
ATOM	1260	CB	LEU	323	62.710	28.740	20.508	1.00	18.36
ATOM	1261	CG	LEU	323	64.179	28.449	20.186	1.00	18.13
ATOM	1262	CD1	LEU	323	64.829	29.669	19.585	1.00	17.37
ATOM	1263	CD2	LEU	323	64.923	27.999	21.447	1.00	17.27
ATOM	1264	C	LEU	323	60.499	28.029	21.454	1.00	18.38
ATOM	1265	O	LEU	323	60.275	28.008	22.663	1.00	18.81
ATOM	1266	N	LEU	324	59.595	28.406	20.557	1.00	18.67
ATOM	1267	CA	LEU	324	58.275	28.897	20.924	1.00	19.02
ATOM	1268	CB	LEU	324	57.564	29.467	19.685	1.00	17.78
ATOM	1269	CG	LEU	324	56.095	29.891	19.838	1.00	17.59
ATOM	1270	CD1	LEU	324	55.983	31.123	20.709	1.00	18.15
ATOM	1271	CD2	LEU	324	55.489	30.180	18.4		

ATOM	1274	N	MET	325	57.224	26.701	21.029	1.00	21.14
ATOM	1275	CA	MET	325	56.330	25.680	21.585	1.00	24.06
ATOM	1276	CB	MET	325	55.857	24.738	20.473	1.00	24.68
ATOM	1277	CG	MET	325	55.169	25.444	19.303	1.00	24.49
ATOM	1278	SD	MET	325	53.759	26.457	19.820	1.00	26.18
ATOM	1279	CE	MET	325	52.609	25.252	20.373	1.00	24.03
ATOM	1280	C	MET	325	56.996	24.887	22.705	1.00	26.15
ATOM	1281	O	MET	325	57.021	23.664	22.693	1.00	25.68
ATOM	1282	N	SER	326	57.555	25.593	23.671	1.00	29.34
ATOM	1283	CA	SER	326	58.232	24.938	24.774	1.00	32.40
ATOM	1284	CB	SER	326	59.512	25.701	25.112	1.00	32.12
ATOM	1285	OG	SER	326	60.127	25.173	26.272	1.00	36.86
ATOM	1286	C	SER	326	57.317	24.831	25.996	1.00	34.04
ATOM	1287	O	SER	326	56.532	25.741	26.280	1.00	33.24
ATOM	1288	N	THR	327	57.366	23.687	26.674	1.00	35.62
ATOM	1289	CA	THR	327	56.560	23.486	27.867	1.00	36.88
ATOM	1290	CB	THR	327	55.938	22.085	27.907	1.00	36.58
ATOM	1291	OG1	THR	327	56.953	21.094	27.714	1.00	38.58
ATOM	1292	CG2	THR	327	54.883	21.938	26.826	1.00	37.73
ATOM	1293	C	THR	327	57.378	23.733	29.135	1.00	38.77
ATOM	1294	O	THR	327	56.921	23.438	30.240	1.00	39.53
ATOM	1295	N	ASP	328	58.593	24.260	28.972	1.00	41.25
ATOM	1296	CA	ASP	328	59.473	24.573	30.099	1.00	43.20
ATOM	1297	CB	ASP	328	60.940	24.698	29.655	1.00	46.47
ATOM	1298	CG	ASP	328	61.618	23.346	29.439	1.00	51.94
ATOM	1299	OD1	ASP	328	62.547	23.278	28.601	1.00	55.43
ATOM	1300	OD2	ASP	328	61.251	22.354	30.111	1.00	54.77
ATOM	1301	C	ASP	328	59.001	25.905	30.653	1.00	43.79
ATOM	1302	O	ASP	328	59.755	26.877	30.709	1.00	45.91
ATOM	1303	N	ARG	329	57.724	25.967	30.995	1.00	43.55
ATOM	1304	CA	ARG	329	57.143	27.178	31.542	1.00	43.04
ATOM	1305	CB	ARG	329	56.398	27.997	30.482	1.00	43.87
ATOM	1306	CG	ARG	329	57.258	28.740	29.504	1.00	40.87
ATOM	1307	CD	ARG	329	57.545	27.886	28.314	1.00	39.52
ATOM	1308	NE	ARG	329	58.301	28.643	27.341	1.00	38.90
ATOM	1309	CZ	ARG	329	59.624	28.708	27.313	1.00	40.59
ATOM	1310	NH1	ARG	329	60.359	28.052	28.196	1.00	42.41
ATOM	1311	NH2	ARG	329	60.210	29.466	26.413	1.00	41.87
ATOM	1312	C	ARG	329	56.152	26.817	32.609	1.00	43.00
ATOM	1313	O	ARG	329	55.600	25.716	32.628	1.00	43.66
ATOM	1314	N	SER	330	55.886	27.797	33.456	1.00	41.58
ATOM	1315	CA	SER	330	54.953	27.641	34.538	1.00	40.11
ATOM	1316	CB	SER	330	55.491	28.362	35.777	1.00	40.38
ATOM	1317	C	SER	330	53.602	28.223	34.103	1.00	38.99
ATOM	1318	O	SER	330	53.553	29.172	33.320	1.00	39.22
ATOM	1								

ATOM	1321	C	GLY	331	50.493	27.782	32.906	1.00	35.14
ATOM	1322	O	GLY	331	49.439	28.363	32.640	1.00	34.48
ATOM	1323	N	LEU	332	51.059	26.925	32.066	1.00	34.54
ATOM	1324	CA	LEU	332	50.424	26.637	30.780	1.00	34.59
ATOM	1325	CB	LEU	332	51.394	25.942	29.828	1.00	33.09
ATOM	1326	CG	LEU	332	52.532	26.765	29.236	1.00	32.72
ATOM	1327	CD1	LEU	332	53.473	25.834	28.497	1.00	30.29
ATOM	1328	CD2	LEU	332	51.987	27.844	28.313	1.00	29.20
ATOM	1329	C	LEU	332	49.191	25.763	30.969	1.00	35.14
ATOM	1330	O	LEU	332	49.178	24.874	31.811	1.00	35.96
ATOM	1331	N	LEU	333	48.153	26.076	30.204	1.00	35.65
ATOM	1332	CA	LEU	333	46.898	25.345	30.215	1.00	37.97
ATOM	1333	CB	LEU	333	45.743	26.271	29.796	1.00	40.71
ATOM	1334	CG	LEU	333	45.389	27.483	30.670	1.00	43.46
ATOM	1335	CD1	LEU	333	44.713	28.620	29.882	1.00	42.72
ATOM	1336	CD2	LEU	333	44.487	27.021	31.806	1.00	45.25
ATOM	1337	C	LEU	333	46.952	24.115	29.300	1.00	37.78
ATOM	1338	O	LEU	333	46.695	22.991	29.720	1.00	37.65
ATOM	1339	N	CYA	334	47.361	24.323	28.060	1.00	38.65
ATOM	1340	CA	CYA	334	47.413	23.249	27.073	1.00	40.91
ATOM	1341	CB	CYA	334	46.936	23.788	25.721	1.00	47.35
ATOM	1342	SG	CYA	334	45.406	24.693	25.867	1.00	52.24
ATOM	1343	AS	CYA	334	44.066	22.890	25.562	1.00	70.72
ATOM	1344	C	CYA	334	48.778	22.588	26.901	1.00	39.85
ATOM	1345	O	CYA	334	49.287	22.473	25.775	1.00	39.54
ATOM	1346	N	VAL	335	49.329	22.078	27.997	1.00	37.67
ATOM	1347	CA	VAL	335	50.641	21.432	27.967	1.00	36.07
ATOM	1348	CB	VAL	335	51.019	20.905	29.384	1.00	33.70
ATOM	1349	CG1	VAL	335	52.434	20.332	29.401	1.00	33.70
ATOM	1350	CG2	VAL	335	50.913	22.028	30.387	1.00	31.84
ATOM	1351	C	VAL	335	50.734	20.334	26.885	1.00	36.09
ATOM	1352	O	VAL	335	51.662	20.335	26.064	1.00	34.41
ATOM	1353	N	ASP	336	49.747	19.444	26.833	1.00	35.95
ATOM	1354	CA	ASP	336	49.748	18.372	25.844	1.00	36.34
ATOM	1355	CB	ASP	336	48.591	17.394	26.091	1.00	41.36
ATOM	1356	CG	ASP	336	48.613	16.206	25.129	1.00	46.23
ATOM	1357	OD1	ASP	336	47.615	16.021	24.392	1.00	49.55
ATOM	1358	OD2	ASP	336	49.639	15.470	25.097	1.00	48.07
ATOM	1359	C	ASP	336	49.727	18.846	24.390	1.00	33.05
ATOM	1360	O	ASP	336	50.527	18.377	23.573	1.00	32.33
ATOM	1361	N	LYS	337	48.794	19.743	24.076	1.00	29.57
ATOM	1362	CA	LYS	337	48.661	20.286	22.723	1.00	27.76
ATOM	1363	CB	LYS	337	47.520	21.313	22.689	1.00	27.09
ATOM	1364	C	LYS	337	49.988	20.941	22.286	1.00	27.64
ATOM	1365	O	LYS	337	50.472	20.713	21.173	1.00	



ATOM	1368	CB	ILE	338	52.128	23.391	24.122	1.00	23.30
ATOM	1369	CG2	ILE	338	53.500	24.048	23.958	1.00	21.75
ATOM	1370	CG1	ILE	338	51.014	24.448	24.155	1.00	21.19
ATOM	1371	CD1	ILE	338	51.055	25.393	25.361	1.00	21.39
ATOM	1372	C	ILE	338	53.041	21.451	22.782	1.00	25.55
ATOM	1373	O	ILE	338	53.861	21.640	21.875	1.00	24.74
ATOM	1374	N	GLU	339	53.124	20.421	23.622	1.00	27.43
ATOM	1375	CA	GLU	339	54.220	19.448	23.536	1.00	27.60
ATOM	1376	CB	GLU	339	54.201	18.512	24.755	1.00	27.21
ATOM	1377	C	GLU	339	54.112	18.650	22.236	1.00	26.85
ATOM	1378	O	GLU	339	55.119	18.385	21.581	1.00	26.71
ATOM	1379	N	LYS	340	52.888	18.276	21.872	1.00	27.04
ATOM	1380	CA	LYS	340	52.663	17.515	20.654	1.00	28.19
ATOM	1381	CB	LYS	340	51.210	17.008	20.609	1.00	28.67
ATOM	1382	C	LYS	340	53.002	18.402	19.439	1.00	27.96
ATOM	1383	O	LYS	340	53.558	17.934	18.436	1.00	27.48
ATOM	1384	N	SER	341	52.746	19.700	19.567	1.00	28.32
ATOM	1385	CA	SER	341	53.058	20.662	18.514	1.00	28.02
ATOM	1386	CB	SER	341	52.457	22.022	18.867	1.00	31.25
ATOM	1387	OG	SER	341	52.880	23.029	17.965	1.00	37.69
ATOM	1388	C	SER	341	54.578	20.773	18.350	1.00	26.01
ATOM	1389	O	SER	341	55.096	20.717	17.234	1.00	25.06
ATOM	1390	N	GLN	342	55.297	20.899	19.462	1.00	25.71
ATOM	1391	CA	GLN	342	56.750	20.993	19.398	1.00	26.39
ATOM	1392	CB	GLN	342	57.356	21.254	20.777	1.00	24.17
ATOM	1393	CG	GLN	342	58.834	21.590	20.703	1.00	25.09
ATOM	1394	CD	GLN	342	59.476	21.677	22.057	1.00	26.93
ATOM	1395	OE1	GLN	342	59.479	20.704	22.810	1.00	27.77
ATOM	1396	NE2	GLN	342	60.022	22.839	22.386	1.00	24.61
ATOM	1397	C	GLN	342	57.354	19.715	18.806	1.00	25.69
ATOM	1398	O	GLN	342	58.356	19.771	18.075	1.00	24.99
ATOM	1399	N	GLU	343	56.753	18.569	19.127	1.00	25.00
ATOM	1400	CA	GLU	343	57.222	17.280	18.610	1.00	25.34
ATOM	1401	CB	GLU	343	56.411	16.118	19.245	1.00	25.90
ATOM	1402	C	GLU	343	57.089	17.276	17.076	1.00	24.32
ATOM	1403	O	GLU	343	58.021	16.891	16.365	1.00	23.99
ATOM	1404	N	ALA	344	55.961	17.789	16.587	1.00	23.56
ATOM	1405	CA	ALA	344	55.701	17.875	15.153	1.00	22.85
ATOM	1406	CB	ALA	344	54.320	18.451	14.917	1.00	22.64
ATOM	1407	C	ALA	344	56.768	18.743	14.489	1.00	22.77
ATOM	1408	O	ALA	344	57.355	18.360	13.477	1.00	22.08
ATOM	1409	N	TYR	345	57.057	19.893	15.092	1.00	21.89
ATOM	1410	CA	TYR	345	58.075	20.792	14.550	1.00	21.18
ATOM	1411	CB	TYR	345	58.108	22.119	15.313	1.00	20.27
ATOM	1412	CG	TYR	345	57.048	23.078	14.856	1.00	



ATOM	1415	CD2 TYR	345	57.063	23.589	13.562	1.00	19.11
ATOM	1416	CE2 TYR	345	56.055	24.424	13.116	1.00	19.14
ATOM	1417	CZ TYR	345	55.017	24.749	13.972	1.00	20.78
ATOM	1418	OH TYR	345	53.983	25.539	13.530	1.00	20.70
ATOM	1419	C TYR	345	59.454	20.167	14.583	1.00	20.96
ATOM	1420	O <sup>-</sup> TYR	345	60.221	20.314	13.632	1.00	22.29
ATOM	1421	N LEU	346	59.778	19.480	15.677	1.00	20.82
ATOM	1422	CA LEU	346	61.079	18.838	15.817	1.00	20.18
ATOM	1423	CB LEU	346	61.216	18.203	17.205	1.00	21.04
ATOM	1424	CG LEU	346	61.606	19.158	18.335	1.00	21.25
ATOM	1425	CD1 LEU	346	61.226	18.595	19.685	1.00	20.95
ATOM	1426	CD2 LEU	346	63.099	19.438	18.267	1.00	19.90
ATOM	1427	C LEU	346	61.317	17.806	14.716	1.00	20.19
ATOM	1428	O LEU	346	62.407	17.755	14.142	1.00	20.69
ATOM	1429	N LEU	347	60.290	17.016	14.390	1.00	22.00
ATOM	1430	CA LEU	347	60.406	15.994	13.344	1.00	21.81
ATOM	1431	CB LEU	347	59.199	15.051	13.366	1.00	24.03
ATOM	1432	CG LEU	347	59.301	13.805	14.250	1.00	26.28
ATOM	1433	CD1 LEU	347	57.964	13.072	14.277	1.00	27.79
ATOM	1434	CD2 LEU	347	60.409	12.889	13.728	1.00	24.78
ATOM	1435	C LEU	347	60.544	16.623	11.966	1.00	20.50
ATOM	1436	O LEU	347	61.351	16.179	11.143	1.00	21.39
ATOM	1437	N ALA	348	59.767	17.674	11.727	1.00	20.84
ATOM	1438	CA ALA	348	59.788	18.381	10.456	1.00	18.12
ATOM	1439	CB ALA	348	58.729	19.480	10.457	1.00	18.49
ATOM	1440	C ALA	348	61.168	18.963	10.269	1.00	17.53
ATOM	1441	O ALA	348	61.785	18.781	9.228	1.00	18.78
ATOM	1442	N PHE	349	61.677	19.569	11.338	1.00	19.55
ATOM	1443	CA PHE	349	63.001	20.196	11.389	1.00	19.84
ATOM	1444	CB PHE	349	63.188	20.823	12.786	1.00	18.68
ATOM	1445	CG PHE	349	64.380	21.758	12.917	1.00	19.12
ATOM	1446	CD1 PHE	349	65.234	22.008	11.851	1.00	19.95
ATOM	1447	CD2 PHE	349	64.618	22.420	14.126	1.00	20.06
ATOM	1448	CE1 PHE	349	66.294	22.905	11.971	1.00	18.99
ATOM	1449	CE2 PHE	349	65.674	23.317	14.261	1.00	16.79
ATOM	1450	CZ PHE	349	66.516	23.562	13.184	1.00	18.91
ATOM	1451	C PHE	349	64.108	19.170	11.103	1.00	20.44
ATOM	1452	O PHE	349	64.980	19.401	10.260	1.00	19.83
ATOM	1453	N GLU	350	64.064	18.032	11.794	1.00	23.59
ATOM	1454	CA GLU	350	65.077	16.995	11.610	1.00	23.46
ATOM	1455	CB GLU	350	64.830	15.845	12.584	1.00	25.26
ATOM	1456	CG GLU	350	65.694	14.644	12.288	1.00	31.98
ATOM	1457	CD GLU	350	65.526	13.482	13.257	1.00	35.49
ATOM	1458	OE1 GLU	350	66.560	12.853	13.555	1.00	40.26
ATOM	1459	OE2 GLU	350	64.380	13.173	13.689	1.00	36.23
ATOM	1460	C GLU	350	65.083	16.489	10.165	1.00	21.12
ATOM	1461	O GLU	350	66.133	16.384	9.526	1.00	19.81

ATOM	1462	N	HIS	351	63.888	16.234	9.651	1.00	21.98
ATOM	1463	CA	HIS	351	63.694	15.751	8.292	1.00	21.31
ATOM	1464	CB	HIS	351	62.238	15.321	8.107	1.00	21.76
ATOM	1465	CG	HIS	351	61.839	14.160	8.967	1.00	22.08
ATOM	1466	CD2	HIS	351	62.578	13.317	9.728	1.00	22.65
ATOM	1467	ND1	HIS	351	60.532	13.751	9.115	1.00	22.37
ATOM	1468	CE1	HIS	351	60.478	12.716	9.930	1.00	21.44
ATOM	1469	NE2	HIS	351	61.705	12.429	10.314	1.00	20.85
ATOM	1470	C	HIS	351	64.117	16.815	7.275	1.00	21.18
ATOM	1471	O	HIS	351	64.683	16.489	6.231	1.00	22.65
ATOM	1472	N	TYR	352	63.915	18.088	7.602	1.00	19.79
ATOM	1473	CA	TYR	352	64.327	19.146	6.697	1.00	18.72
ATOM	1474	CB	TYR	352	63.768	20.502	7.122	1.00	19.55
ATOM	1475	CG	TYR	352	64.140	21.580	6.137	1.00	19.27
ATOM	1476	CD1	TYR	352	63.556	21.623	4.867	1.00	19.29
ATOM	1477	CE1	TYR	352	63.961	22.555	3.927	1.00	17.55
ATOM	1478	CD2	TYR	352	65.132	22.507	6.438	1.00	18.91
ATOM	1479	CE2	TYR	352	65.545	23.443	5.503	1.00	17.30
ATOM	1480	CZ	TYR	352	64.954	23.459	4.256	1.00	18.41
ATOM	1481	OH	TYR	352	65.355	24.384	3.334	1.00	19.40
ATOM	1482	C	TYR	352	65.849	19.182	6.687	1.00	19.31
ATOM	1483	O	TYR	352	66.479	19.333	5.639	1.00	20.25
ATOM	1484	N	VAL	353	66.446	19.017	7.858	1.00	21.25
ATOM	1485	CA	VAL	353	67.899	18.993	7.960	1.00	22.03
ATOM	1486	CB	VAL	353	68.348	18.880	9.450	1.00	22.60
ATOM	1487	CG1	VAL	353	69.843	18.635	9.550	1.00	20.34
ATOM	1488	CG2	VAL	353	67.997	20.167	10.183	1.00	22.61
ATOM	1489	C	VAL	353	68.442	17.827	7.108	1.00	22.74
ATOM	1490	O	VAL	353	69.448	17.985	6.398	1.00	23.44
ATOM	1491	N	ASN	354	67.773	16.674	7.165	1.00	22.30
ATOM	1492	CA	ASN	354	68.185	15.508	6.373	1.00	23.56
ATOM	1493	CB	ASN	354	67.241	14.320	6.603	1.00	22.26
ATOM	1494	CG	ASN	354	67.374	13.715	7.981	1.00	23.06
ATOM	1495	OD1	ASN	354	68.406	13.843	8.628	1.00	25.79
ATOM	1496	ND2	ASN	354	66.327	13.044	8.435	1.00	21.07
ATOM	1497	C	ASN	354	68.134	15.877	4.888	1.00	25.10
ATOM	1498	O	ASN	354	69.024	15.534	4.111	1.00	26.70
ATOM	1499	N	HIS	355	67.067	16.568	4.503	1.00	24.50
ATOM	1500	CA	HIS	355	66.881	16.986	3.123	1.00	24.46
ATOM	1501	CB	HIS	355	65.557	17.750	2.969	1.00	26.07
ATOM	1502	CG	HIS	355	65.365	18.337	1.604	1.00	28.28
ATOM	1503	CD2	HIS	355	65.918	19.422	1.018	1.00	28.10
ATOM	1504	ND1	HIS	355	64.600	17.724	0.632	1.00	26.32
ATOM	1505	CE1	HIS	355	64.706	18.407	-0.499	1.00	27.71
ATOM	1506	NE2	HIS	355	65.502	19.435	-0.288	1.00	27.79
ATOM	1507	C	HIS						

ATOM	1509	N	ARG	356	68.463	18.774	3.471	1.00	25.31
ATOM	1510	CA	ARG	356	69.523	19.714	3.130	1.00	25.69
ATOM	1511	CB	ARG	356	69.561	20.820	4.168	1.00	24.06
ATOM	1512	CG	ARG	356	68.337	21.682	4.094	1.00	23.23
ATOM	1513	CD	ARG	356	68.670	22.973	3.424	1.00	25.91
ATOM	1514	NE	ARG	356	69.447	23.814	4.322	1.00	24.87
ATOM	1515	CZ	ARG	356	70.325	24.726	3.928	1.00	25.05
ATOM	1516	NH1	ARG	356	70.546	24.920	2.640	1.00	24.97
ATOM	1517	NH2	ARG	356	70.978	25.453	4.831	1.00	25.62
ATOM	1518	C	ARG	356	70.900	19.109	2.949	1.00	27.73
ATOM	1519	O	ARG	356	71.724	19.645	2.208	1.00	28.38
ATOM	1520	N	LYS	357	71.179	18.048	3.693	1.00	29.45
ATOM	1521	CA	LYS	357	72.457	17.355	3.588	1.00	31.35
ATOM	1522	CB	LYS	357	72.503	16.566	2.270	1.00	32.80
ATOM	1523	CG	LYS	357	71.290	15.650	2.103	1.00	35.78
ATOM	1524	CD	LYS	357	71.264	14.927	0.778	1.00	39.43
ATOM	1525	CE	LYS	357	70.121	13.918	0.739	1.00	42.93
ATOM	1526	NZ	LYS	357	70.162	13.074	-0.498	1.00	45.97
ATOM	1527	C	LYS	357	73.692	18.247	3.743	1.00	31.34
ATOM	1528	O	LYS	357	74.489	18.390	2.818	1.00	32.65
ATOM	1529	N	HIS	358	73.837	18.861	4.913	1.00	30.72
ATOM	1530	CA	HIS	358	74.995	19.706	5.186	1.00	31.49
ATOM	1531	CB	HIS	358	74.895	20.322	6.579	1.00	29.13
ATOM	1532	CG	HIS	358	73.882	21.415	6.688	1.00	25.30
ATOM	1533	CD2	HIS	358	74.026	22.760	6.646	1.00	24.90
ATOM	1534	ND1	HIS	358	72.543	21.175	6.892	1.00	24.54
ATOM	1535	CE1	HIS	358	71.901	22.324	6.975	1.00	23.68
ATOM	1536	NE2	HIS	358	72.777	23.302	6.830	1.00	25.28
ATOM	1537	C	HIS	358	76.235	18.831	5.161	1.00	33.38
ATOM	1538	O	HIS	358	76.166	17.647	5.495	1.00	35.46
ATOM	1539	N	ASN	359	77.366	19.399	4.768	1.00	35.34
ATOM	1540	CA	ASN	359	78.606	18.636	4.746	1.00	38.17
ATOM	1541	CB	ASN	359	79.544	19.150	3.646	1.00	37.84
ATOM	1542	C	ASN	359	79.236	18.825	6.120	1.00	39.85
ATOM	1543	O	ASN	359	80.317	19.406	6.240	1.00	42.72
ATOM	1544	N	ILE	360	78.510	18.411	7.159	1.00	39.01
ATOM	1545	CA	ILE	360	78.968	18.526	8.549	1.00	36.72
ATOM	1546	CB	ILE	360	78.351	19.752	9.264	1.00	37.69
ATOM	1547	CG2	ILE	360	78.802	19.793	10.722	1.00	37.56
ATOM	1548	CG1	ILE	360	78.735	21.049	8.549	1.00	37.68
ATOM	1549	CD1	ILE	360	77.970	22.253	9.041	1.00	38.40
ATOM	1550	C	ILE	360	78.524	17.278	9.303	1.00	35.15
ATOM	1551	O	ILE	360	77.343	16.931	9.314	1.00	33.75
ATOM	1552	N	PRO	361	79.475	16.564	9.912	1.00	34.64
ATOM	1553	CD	PRO	361	80.930	16.785	9.873	1.00	35.59
ATOM	1554	CA	PRO	361	79				

ATOM	1556	CG	PRO	361	81.412	15.972	11.048	1.00	35.97
ATOM	1557	C	PRO	361	78.292	15.618	11.909	1.00	30.95
ATOM	1558	O	PRO	361	78.555	16.554	12.653	1.00	31.50
ATOM	1559	N	HIS	362	77.269	14.793	12.112	1.00	28.75
ATOM	1560	CA	HIS	362	76.378	14.900	13.263	1.00	30.25
ATOM	1561	CB	HIS	362	77.152	14.612	14.548	1.00	31.20
ATOM	1562	CG	HIS	362	78.075	13.441	14.440	1.00	33.72
ATOM	1563	CD2	HIS	362	77.826	12.122	14.275	1.00	34.55
ATOM	1564	ND1	HIS	362	79.449	13.569	14.469	1.00	35.55
ATOM	1565	CE1	HIS	362	80.006	12.377	14.322	1.00	35.28
ATOM	1566	NE2	HIS	362	79.040	11.484	14.204	1.00	37.61
ATOM	1567	C	HIS	362	75.742	16.275	13.368	1.00	29.44
ATOM	1568	O	HIS	362	75.521	16.769	14.472	1.00	29.93
ATOM	1569	N	PHE	363	75.397	16.856	12.222	1.00	29.22
ATOM	1570	CA	PHE	363	74.803	18.188	12.160	1.00	27.72
ATOM	1571	CB	PHE	363	74.446	18.538	10.709	1.00	26.85
ATOM	1572	CG	PHE	363	73.901	19.931	10.532	1.00	27.48
ATOM	1573	CD1	PHE	363	74.758	21.017	10.391	1.00	27.76
ATOM	1574	CD2	PHE	363	72.523	20.157	10.513	1.00	27.45
ATOM	1575	CE1	PHE	363	74.244	22.313	10.234	1.00	28.56
ATOM	1576	CE2	PHE	363	72.001	21.446	10.357	1.00	25.15
ATOM	1577	CZ	PHE	363	72.860	22.521	10.219	1.00	24.41
ATOM	1578	C	PHE	363	73.597	18.385	13.075	1.00	27.45
ATOM	1579	O	PHE	363	73.577	19.324	13.880	1.00	27.73
ATOM	1580	N	TRP	364	72.616	17.489	12.983	1.00	25.89
ATOM	1581	CA	TRP	364	71.401	17.592	13.800	1.00	25.85
ATOM	1582	CB	TRP	364	70.444	16.426	13.506	1.00	24.27
ATOM	1583	CG	TRP	364	69.168	16.391	14.328	1.00	23.75
ATOM	1584	CD2	TRP	364	68.152	17.407	14.397	1.00	24.87
ATOM	1585	CE2	TRP	364	67.140	16.922	15.261	1.00	24.81
ATOM	1586	CE3	TRP	364	67.989	18.674	13.820	1.00	25.47
ATOM	1587	CD1	TRP	364	68.745	15.370	15.122	1.00	22.98
ATOM	1588	NE1	TRP	364	67.530	15.679	15.684	1.00	25.99
ATOM	1589	CZ2	TRP	364	65.987	17.661	15.560	1.00	25.14
ATOM	1590	CZ3	TRP	364	66.844	19.405	14.116	1.00	25.29
ATOM	1591	CH2	TRP	364	65.857	18.894	14.982	1.00	24.53
ATOM	1592	C	TRP	364	71.659	17.747	15.308	1.00	26.94
ATOM	1593	O	TRP	364	71.202	18.721	15.904	1.00	27.16
ATOM	1594	N	PRO	365	72.382	16.796	15.944	1.00	27.60
ATOM	1595	CD	PRO	365	72.912	15.522	15.411	1.00	27.55
ATOM	1596	CA	PRO	365	72.655	16.915	17.387	1.00	25.90
ATOM	1597	CB	PRO	365	73.565	15.717	17.668	1.00	26.00
ATOM	1598	CG	PRO	365	73.136	14.705	16.658	1.00	28.32
ATOM	1599	C	PRO	365	73.374	18.225	17.714	1.00	23.89
ATOM	1600	O	PRO	365	73.088	18.861	18.725	1.	



ATOM	1603	CB	LYS	366	76.144	19.982	15.963	1.00	27.44
ATOM	1604	CG	LYS	366	77.310	19.022	16.138	1.00	28.76
ATOM	1605	CD	LYS	366	78.254	19.171	14.975	1.00	30.53
ATOM	1606	CE	LYS	366	79.527	18.387	15.167	1.00	34.25
ATOM	1607	NZ	LYS	366	80.388	18.463	13.947	1.00	37.89
ATOM	1608	C <sup>-</sup>	LYS	366	74.181	21.107	16.993	1.00	26.73
ATOM	1609	O	LYS	366	74.385	22.042	17.762	1.00	27.36
ATOM	1610	N	LEU	367	73.216	21.124	16.086	1.00	27.98
ATOM	1611	CA	LEU	367	72.308	22.256	15.967	1.00	27.87
ATOM	1612	CB	LEU	367	71.559	22.192	14.632	1.00	27.29
ATOM	1613	CG	LEU	367	70.613	23.356	14.318	1.00	27.25
ATOM	1614	CD1	LEU	367	71.334	24.707	14.510	1.00	22.90
ATOM	1615	CD2	LEU	367	70.081	23.189	12.896	1.00	24.54
ATOM	1616	C	LEU	367	71.327	22.223	17.134	1.00	29.38
ATOM	1617	O	LEU	367	70.993	23.249	17.716	1.00	31.09
ATOM	1618	N	LEU	368	70.889	21.026	17.491	1.00	30.38
ATOM	1619	CA	LEU	368	69.962	20.843	18.594	1.00	31.14
ATOM	1620	CB	LEU	368	69.659	19.353	18.731	1.00	32.20
ATOM	1621	CG	LEU	368	68.247	18.852	19.014	1.00	33.52
ATOM	1622	CD1	LEU	368	67.184	19.651	18.267	1.00	31.14
ATOM	1623	CD2	LEU	368	68.210	17.379	18.632	1.00	33.99
ATOM	1624	C	LEU	368	70.601	21.395	19.876	1.00	32.36
ATOM	1625	O	LEU	368	69.917	21.963	20.730	1.00	32.58
ATOM	1626	N	MET	369	71.922	21.272	19.985	1.00	33.30
ATOM	1627	CA	MET	369	72.641	21.771	21.149	1.00	34.04
ATOM	1628	CB	MET	369	74.051	21.190	21.209	1.00	35.31
ATOM	1629	CG	MET	369	74.108	19.858	21.935	1.00	36.83
ATOM	1630	SD	MET	369	75.312	18.728	21.235	1.00	43.07
ATOM	1631	CE	MET	369	76.862	19.636	21.472	1.00	41.31
ATOM	1632	C	MET	369	72.675	23.297	21.212	1.00	34.30
ATOM	1633	O	MET	369	72.961	23.876	22.269	1.00	35.82
ATOM	1634	N	LYS	370	72.368	23.949	20.091	1.00	32.14
ATOM	1635	CA	LYS	370	72.325	25.405	20.044	1.00	29.17
ATOM	1636	CB	LYS	370	72.394	25.904	18.608	1.00	28.18
ATOM	1637	CG	LYS	370	73.662	25.518	17.900	1.00	27.72
ATOM	1638	CD	LYS	370	74.866	25.969	18.679	1.00	28.10
ATOM	1639	CE	LYS	370	76.127	25.650	17.930	1.00	27.79
ATOM	1640	NZ	LYS	370	77.298	25.941	18.777	1.00	30.78
ATOM	1641	C	LYS	370	71.033	25.875	20.705	1.00	29.27
ATOM	1642	O	LYS	370	70.950	26.999	21.200	1.00	29.43
ATOM	1643	N	VAL	371	70.018	25.014	20.714	1.00	29.40
ATOM	1644	CA	VAL	371	68.756	25.358	21.358	1.00	29.90
ATOM	1645	CB	VAL	371	67.687	24.237	21.218	1.00	28.75
ATOM	1646	CG1	VAL	371	66.463	24.561	22.064	1.00	27.12
ATOM	1647	CG2	VAL	371	67.275	24.080	1		



ATOM	1650	N	THR	372	69.971	24.743	23.366	1.00	31.39
ATOM	1651	CA	THR	372	70.371	24.847	24.762	1.00	31.10
ATOM	1652	CB	THR	372	71.282	23.664	25.170	1.00	31.59
ATOM	1653	OG1	THR	372	70.554	22.441	25.008	1.00	30.60
ATOM	1654	CG2	THR	372	71.720	23.795	26.625	1.00	30.14
ATOM	1655	C	THR	372	71.071	26.186	24.994	1.00	30.76
ATOM	1656	O	THR	372	70.711	26.935	25.910	1.00	31.45
ATOM	1657	N	ASP	373	72.038	26.507	24.138	1.00	29.31
ATOM	1658	CA	ASP	373	72.744	27.772	24.252	1.00	27.32
ATOM	1659	CB	ASP	373	73.745	27.934	23.115	1.00	27.98
ATOM	1660	CG	ASP	373	74.886	26.933	23.190	1.00	28.94
ATOM	1661	OD1	ASP	373	75.043	26.259	24.225	1.00	31.01
ATOM	1662	OD2	ASP	373	75.639	26.825	22.205	1.00	31.38
ATOM	1663	C	ASP	373	71.742	28.926	24.247	1.00	26.50
ATOM	1664	O	ASP	373	71.872	29.861	25.040	1.00	27.35
ATOM	1665	N	LEU	374	70.711	28.826	23.412	1.00	24.17
ATOM	1666	CA	LEU	374	69.688	29.864	23.331	1.00	23.38
ATOM	1667	CB	LEU	374	68.795	29.660	22.107	1.00	22.98
ATOM	1668	CG	LEU	374	69.361	30.183	20.786	1.00	24.45
ATOM	1669	CD1	LEU	374	68.668	29.520	19.589	1.00	24.72
ATOM	1670	CD2	LEU	374	69.223	31.704	20.735	1.00	22.40
ATOM	1671	C	LEU	374	68.839	29.964	24.589	1.00	24.31
ATOM	1672	O	LEU	374	68.442	31.065	24.986	1.00	23.31
ATOM	1673	N	ARG	375	68.543	28.826	25.211	1.00	25.32
ATOM	1674	CA	ARG	375	67.748	28.821	26.438	1.00	27.76
ATOM	1675	CB	ARG	375	67.455	27.392	26.908	1.00	30.82
ATOM	1676	CG	ARG	375	66.901	26.439	25.854	1.00	38.79
ATOM	1677	CD	ARG	375	65.424	26.630	25.582	1.00	45.40
ATOM	1678	NE	ARG	375	64.709	25.360	25.620	1.00	52.61
ATOM	1679	CZ	ARG	375	63.800	24.967	24.726	1.00	56.89
ATOM	1680	NH1	ARG	375	63.473	25.732	23.694	1.00	58.27
ATOM	1681	NH2	ARG	375	63.201	23.793	24.855	1.00	58.46
ATOM	1682	C	ARG	375	68.563	29.542	27.512	1.00	26.98
ATOM	1683	O	ARG	375	68.025	30.336	28.282	1.00	26.18
ATOM	1684	N	MET	376	69.862	29.255	27.551	1.00	26.80
ATOM	1685	CA	MET	376	70.767	29.867	28.511	1.00	29.22
ATOM	1686	CB	MET	376	72.172	29.270	28.379	1.00	33.70
ATOM	1687	CG	MET	376	72.595	28.371	29.562	1.00	43.20
ATOM	1688	SD	MET	376	73.320	29.260	31.011	1.00	52.38
ATOM	1689	CE	MET	376	71.843	29.854	31.913	1.00	48.11
ATOM	1690	C	MET	376	70.804	31.384	28.339	1.00	27.54
ATOM	1691	O	MET	376	70.792	32.126	29.323	1.00	26.96
ATOM	1692	N	ILE	377	70.841	31.835	27.087	1.00	25.39
ATOM	1693	CA	ILE	377	70.847	33.264	26.767	1.00	23.26
ATOM	1694	CB	ILE	377	70.992	33.488	25.222	1.00	22.73

ATOM	1697	CD1	ILE	377	72.644	33.148	23.300	1.00	18.85
ATOM	1698	C	ILE	377	69.558	33.900	27.309	1.00	22.91
ATOM	1699	O	ILE	377	69.597	34.925	27.989	1.00	22.02
ATOM	1700	N	GLY	378	68.427	33.244	27.069	1.00	22.29
ATOM	1701	CA	GLY	378	67.161	33.757	27.547	1.00	22.83
ATOM	1702	C	GLY	378	67.111	33.815	29.063	1.00	25.60
ATOM	1703	O	GLY	378	66.546	34.752	29.630	1.00	26.25
ATOM	1704	N	ALA	379	67.691	32.804	29.713	1.00	26.88
ATOM	1705	CA	ALA	379	67.744	32.707	31.175	1.00	27.19
ATOM	1706	CB	ALA	379	68.322	31.358	31.590	1.00	26.97
ATOM	1707	C	ALA	379	68.606	33.827	31.738	1.00	26.13
ATOM	1708	O	ALA	379	68.174	34.580	32.601	1.00	26.46
ATOM	1709	N	CYA	380	69.826	33.935	31.230	1.00	27.61
ATOM	1710	CA	CYA	380	70.742	34.973	31.667	1.00	29.74
ATOM	1711	CB	CYA	380	72.070	34.865	30.923	1.00	35.44
ATOM	1712	SG	CYA	380	73.081	33.458	31.417	1.00	42.61
ATOM	1713	AS	CYA	380	74.829	33.691	29.945	1.00	55.91
ATOM	1714	C	CYA	380	70.142	36.349	31.446	1.00	29.07
ATOM	1715	O	CYA	380	70.243	37.225	32.303	1.00	29.46
ATOM	1716	N	HIS	381	69.494	36.538	30.304	1.00	28.29
ATOM	1717	CA	HIS	381	68.885	37.824	30.002	1.00	26.84
ATOM	1718	CB	HIS	381	68.384	37.880	28.557	1.00	23.13
ATOM	1719	CG	HIS	381	67.597	39.113	28.259	1.00	19.84
ATOM	1720	CD2	HIS	381	67.993	40.365	27.931	1.00	18.68
ATOM	1721	ND1	HIS	381	66.229	39.169	28.403	1.00	19.47
ATOM	1722	CE1	HIS	381	65.817	40.407	28.190	1.00	18.64
ATOM	1723	NE2	HIS	381	66.868	41.149	27.900	1.00	18.29
ATOM	1724	C	HIS	381	67.747	38.157	30.967	1.00	26.78
ATOM	1725	O	HIS	381	67.560	39.314	31.337	1.00	26.39
ATOM	1726	N	ALA	382	66.964	37.158	31.347	1.00	27.78
ATOM	1727	CA	ALA	382	65.867	37.395	32.269	1.00	29.45
ATOM	1728	CB	ALA	382	65.077	36.125	32.471	1.00	29.51
ATOM	1729	C	ALA	382	66.425	37.904	33.604	1.00	31.74
ATOM	1730	O	ALA	382	65.932	38.882	34.159	1.00	32.60
ATOM	1731	N	SER	383	67.483	37.262	34.093	1.00	33.02
ATOM	1732	CA	SER	383	68.109	37.662	35.350	1.00	34.69
ATOM	1733	CB	SER	383	69.212	36.677	35.733	1.00	36.18
ATOM	1734	OG	SER	383	68.663	35.386	35.933	1.00	40.61
ATOM	1735	C	SER	383	68.689	39.064	35.242	1.00	33.49
ATOM	1736	O	SER	383	68.526	39.889	36.146	1.00	34.28
ATOM	1737	N	ARG	384	69.377	39.332	34.141	1.00	32.60
ATOM	1738	CA	ARG	384	69.955	40.642	33.938	1.00	32.60
ATOM	1739	CB	ARG	384	70.926	40.638	32.762	1.00	33.60
ATOM	1740	CG	ARG	384	71.429	42.013	32.409	1.00	36.33
ATOM	1741	CD	ARG	384	72.875	41.975	31.993	1.00	39.62
ATOM	1742	NE	ARG	384	73.760	42.260	33.114	1.00	41.76
ATOM	1743	CZ	ARG	384	74.587	43.301	33.179	1.00	41.92

ATOM	1744	NH1	ARG	384	74.670	44.182	32.191	1.00	40.66	
ATOM	1745	NH2	ARG	384	75.319	43.471	34.260	1.00	44.88	
ATOM	1746	C	ARG	384	68.862	41.694	33.758	1.00	32.28	
ATOM	1747	O	ARG	384	69.014	42.831	34.213	1.00	33.27	
ATOM	1748	N	PHE	385	67.739	41.311	33.159	1.00	29.13	
ATOM	1749	CA	PHE	385	66.663	42.259	32.977	1.00	27.55	
ATOM	1750	CB	PHE	385	65.552	41.687	32.105	1.00	26.89	
ATOM	1751	CG	PHE	385	64.415	42.641	31.888	1.00	25.11	
ATOM	1752	CD1	PHE	385	64.495	43.630	30.918	1.00	24.94	
ATOM	1753	CD2	PHE	385	63.281	42.580	32.689	1.00	25.01	
ATOM	1754	CE1	PHE	385	63.466	44.547	30.753	1.00	25.50	
ATOM	1755	CE2	PHE	385	62.244	43.495	32.531	1.00	24.06	
ATOM	1756	CZ	PHE	385	62.338	44.482	31.563	1.00	25.44	
ATOM	1757	C	PHE	385	66.125	42.641	34.348	1.00	29.08	
ATOM	1758	O	PHE	385	65.887	43.816	34.613	1.00	27.90	
ATOM	1759	N	LEU	386	65.972	41.658	35.231	1.00	31.19	
ATOM	1760	CA	LEU	386	65.465	41.929	36.577	1.00	33.22	
ATOM	1761	CB	LEU	386	65.355	40.640	37.397	1.00	34.35	
ATOM	1762	C	LEU	386	66.362	42.940	37.279	1.00	33.52	
ATOM	1763	O	LEU	386	65.874	43.907	37.855	1.00	32.93	
ATOM	1764	N	HIS	387	67.673	42.760	37.158	1.00	34.80	
ATOM	1765	CA	HIS	387	68.628	43.674	37.775	1.00	37.88	
ATOM	1766	CB	HIS	387	70.042	43.112	37.705	1.00	36.66	
ATOM	1767	CG	HIS	387	70.206	41.832	38.456	1.00	39.14	
ATOM	1768	CD2	HIS	387	69.307	41.080	39.144	1.00	39.28	
ATOM	1769	ND1	HIS	387	71.408	41.161	38.543	1.00	40.97	
ATOM	1770	CE1	HIS	387	71.241	40.055	39.245	1.00	41.57	
ATOM	1771	NE2	HIS	387	69.980	39.984	39.618	1.00	41.45	
ATOM	1772	C	HIS	387	68.589	45.071	37.164	1.00	40.38	
ATOM	1773	O	HIS	387	68.673	46.054	37.888	1.00	40.87	
ATOM	1774	N	MET	388	68.466	45.161	35.842	1.00	43.32	
ATOM	1775	CA	MET	388	68.398	46.455	35.168	1.00	46.28	
ATOM	1776	CB	MET	388	68.170	46.286	33.665	1.00	43.30	
ATOM	1777	CG	MET	388	69.342	45.738	32.875	1.00	43.55	
ATOM	1778	SD	MET	388	69.034	45.896	31.098	1.00	46.27	
ATOM	1779	CE	MET	388	68.208	44.370	30.709	1.00	42.36	
ATOM	1780	C	MET	388	67.256	47.289	35.737	1.00	50.25	
ATOM	1781	O	MET	388	67.363	48.506	35.886	1.00	49.79	
ATOM	1782	N	LYS	389	66.163	46.610	36.075	1.00	52.74	ALTA
ATOM	1783	CA	LYS	389	64.983	47.274	36.633	1.00	56.15	ALTA
ATOM	1784	CB	LYS	389	63.770	46.334	36.565	1.00	56.87	ALTA
ATOM	1785	CG	LYS	389	63.227	46.087	35.161	1.00	57.76	ALTA
ATOM	1786	CD	LYS	389	62.029	45.156	35.212	1.00	55.98</	

ATOM	1791	N	VAL	390	65.955	47.038	38.839	1.00	55.21
ATOM	1792	CA	VAL	390	66.225	47.386	40.236	1.00	51.78
ATOM	1793	CB	VAL	390	66.999	46.231	40.985	1.00	50.07
ATOM	1794	CG1	VAL	390	67.648	46.726	42.263	1.00	49.74
ATOM	1795	CG2	VAL	390	66.037	45.093	41.317	1.00	49.06
ATOM	1796	C	VAL	390	67.053	48.681	40.227	1.00	49.38
ATOM	1797	O	VAL	390	66.785	49.605	40.992	1.00	48.71
ATOM	1798	N	GLU	391	67.974	48.778	39.272	1.00	46.71
ATOM	1799	CA	GLU	391	68.866	49.919	39.142	1.00	44.88
ATOM	1800	CB	GLU	391	70.156	49.488	38.438	1.00	45.24
ATOM	1801	CG	GLU	391	70.793	48.207	38.997	1.00	47.65
ATOM	1802	CD	GLU	391	71.461	48.388	40.358	1.00	50.29
ATOM	1803	OE1	GLU	391	71.141	49.373	41.063	1.00	50.68
ATOM	1804	OE2	GLU	391	72.310	47.535	40.718	1.00	50.85
ATOM	1805	C	GLU	391	68.324	51.174	38.458	1.00	45.28
ATOM	1806	O	GLU	391	68.568	52.286	38.940	1.00	46.46
ATOM	1807	N	CYA	392	67.568	51.024	37.372	1.00	43.33
ATOM	1808	CA	CYA	392	67.071	52.192	36.643	1.00	42.28
ATOM	1809	CB	CYA	392	67.519	52.096	35.197	1.00	42.45
ATOM	1810	SG	CYA	392	69.280	52.182	35.127	1.00	43.69
ATOM	1811	AS	CYA	392	69.908	51.044	33.336	1.00	48.17
ATOM	1812	C	CYA	392	65.589	52.493	36.709	1.00	42.51
ATOM	1813	O	CYA	392	64.792	51.634	37.070	1.00	43.30
ATOM	1814	N	PRO	393	65.205	53.752	36.418	1.00	42.13
ATOM	1815	CD	PRO	393	66.109	54.899	36.199	1.00	40.54
ATOM	1816	CA	PRO	393	63.794	54.182	36.441	1.00	42.26
ATOM	1817	CB	PRO	393	63.896	55.710	36.365	1.00	41.47
ATOM	1818	CG	PRO	393	65.189	55.938	35.614	1.00	41.10
ATOM	1819	C	PRO	393	62.954	53.606	35.281	1.00	43.20
ATOM	1820	O	PRO	393	63.463	53.452	34.163	1.00	42.61
ATOM	1821	N	THR	394	61.686	53.305	35.559	1.00	43.70
ATOM	1822	CA	THR	394	60.764	52.755	34.564	1.00	45.50
ATOM	1823	CB	THR	394	59.340	52.609	35.129	1.00	47.20
ATOM	1824	OG1	THR	394	59.304	53.139	36.464	1.00	50.57
ATOM	1825	CG2	THR	394	58.878	51.150	35.137	1.00	47.99
ATOM	1826	C	THR	394	60.682	53.583	33.283	1.00	44.58
ATOM	1827	O	THR	394	60.409	53.054	32.215	1.00	46.36
ATOM	1828	N	GLU	395	60.899	54.888	33.396	1.00	42.88
ATOM	1829	CA	GLU	395	60.842	55.790	32.246	1.00	40.54
ATOM	1830	CB	GLU	395	61.096	57.234	32.699	1.00	40.69
ATOM	1831	C	GLU	395	61.799	55.421	31.098	1.00	38.51
ATOM	1832	O	GLU	395	61.628	55.877	29.968	1.00	39.41
ATOM	1833	N	LEU	396	62.828	54.640	31.402	1.00	35.60
ATOM	1834	CA	LEU	396	63.795	54.220	30.386	1.00	33.11
ATOM	1835	CB	LEU	396	65.169	54.003	31.027	1.00	33.60



ATOM	1838	CD2 LEU	396	66.026	56.308	30.599	1.00	35.71
ATOM	1839	C LEU	396	63.388	52.940	29.660	1.00	30.95
ATOM	1840	O LEU	396	63.950	52.605	28.624	1.00	30.90
ATOM	1841	N PHE	397	62.422	52.227	30.223	1.00	30.18
ATOM	1842	CA PHE	397	61.961	50.970	29.654	1.00	28.80
ATOM	1843	CB PHE	397	61.712	49.946	30.777	1.00	28.10
ATOM	1844	CG PHE	397	62.938	49.604	31.592	1.00	28.96
ATOM	1845	CD1 PHE	397	63.403	50.472	32.591	1.00	28.39
ATOM	1846	CD2 PHE	397	63.636	48.422	31.359	1.00	26.28
ATOM	1847	CE1 PHE	397	64.546	50.166	33.337	1.00	28.44
ATOM	1848	CE2 PHE	397	64.784	48.107	32.103	1.00	29.21
ATOM	1849	CZ PHE	397	65.240	48.984	33.096	1.00	27.37
ATOM	1850	C PHE	397	60.683	51.093	28.836	1.00	27.54
ATOM	1851	O PHE	397	59.630	51.431	29.370	1.00	26.96
ATOM	1852	N PRO	398	60.753	50.836	27.501	1.00	27.41
ATOM	1853	CD PRO	398	61.968	50.600	26.686	1.00	25.42
ATOM	1854	CA PRO	398	59.560	50.920	26.654	1.00	25.90
ATOM	1855	CB PRO	398	60.068	50.383	25.320	1.00	25.26
ATOM	1856	CG PRO	398	61.490	50.893	25.290	1.00	23.99
ATOM	1857	C PRO	398	58.494	49.995	27.272	1.00	25.86
ATOM	1858	O PRO	398	58.839	48.962	27.843	1.00	25.82
ATOM	1859	N PRO	399	57.197	50.355	27.175	1.00	25.52
ATOM	1860	CD PRO	399	56.627	51.576	26.578	1.00	25.49
ATOM	1861	CA PRO	399	56.145	49.510	27.754	1.00	25.42
ATOM	1862	CB PRO	399	54.861	50.181	27.273	1.00	26.23
ATOM	1863	CG PRO	399	55.237	51.609	27.156	1.00	25.25
ATOM	1864	C PRO	399	56.198	48.043	27.317	1.00	26.08
ATOM	1865	O PRO	399	56.132	47.131	28.159	1.00	25.45
ATOM	1866	N LEU	400	56.350	47.810	26.019	1.00	25.57
ATOM	1867	CA LEU	400	56.406	46.440	25.509	1.00	26.27
ATOM	1868	CB LEU	400	56.404	46.418	23.980	1.00	25.03
ATOM	1869	CG LEU	400	56.117	45.042	23.363	1.00	24.51
ATOM	1870	CD1 LEU	400	54.757	44.530	23.806	1.00	23.22
ATOM	1871	CD2 LEU	400	56.173	45.149	21.862	1.00	23.70
ATOM	1872	C LEU	400	57.602	45.657	26.067	1.00	27.06
ATOM	1873	O LEU	400	57.484	44.465	26.363	1.00	27.41
ATOM	1874	N PHE	401	58.736	46.339	26.231	1.00	27.16
ATOM	1875	CA PHE	401	59.966	45.754	26.779	1.00	27.06
ATOM	1876	CB PHE	401	61.047	46.833	26.802	1.00	26.60
ATOM	1877	CG PHE	401	62.408	46.351	27.217	1.00	28.08
ATOM	1878	CD1 PHE	401	62.918	45.138	26.747	1.00	27.45
ATOM	1879	CD2 PHE	401	63.223	47.165	28.013	1.00	27.48
ATOM	1880	CE1 PHE	401	64.220	44.746	27.055	1.00	26.95
ATOM	1881	CE2 PHE	401	64.523	46.786	28.327	1.00	27.97
ATOM	1882	CZ PHE	401	65.028	45.575	27.846	1.00	28.46
ATOM	1883	C PHE	401	59.690	45.247	28.205	1.00	27.62
ATOM	1884	O PHE	401	60.046	44.125	28.570	1.00	26.24



ATOM	1885	N	LEU	402	59.036	46.082	29.002	1.00	28.75	
ATOM	1886	CA	LEU	402	58.692	45.719	30.366	1.00	29.58	
ATOM	1887	CB	LEU	402	58.064	46.910	31.088	1.00	30.04	
ATOM	1888	CG	LEU	402	59.025	47.974	31.594	1.00	30.14	
ATOM	1889	CD1	LEU	402	58.270	49.263	31.880	1.00	29.61	
ATOM	1890	CD2	LEU	402	59.734	47.438	32.827	1.00	27.99	
ATOM	1891	C	LEU	402	57.693	44.583	30.368	1.00	30.10	
ATOM	1892	O	LEU	402	57.836	43.631	31.121	1.00	29.78	
ATOM	1893	N	GLU	403	56.688	44.683	29.510	1.00	30.49	
ATOM	1894	CA	GLU	403	55.646	43.671	29.453	1.00	32.60	
ATOM	1895	CB	GLU	403	54.562	44.094	28.469	1.00	37.01	
ATOM	1896	CG	GLU	403	53.329	43.218	28.520	1.00	44.01	
ATOM	1897	CD	GLU	403	52.263	43.632	27.523	1.00	48.50	
ATOM	1898	OE1	GLU	403	52.516	44.525	26.677	1.00	49.66	
ATOM	1899	OE2	GLU	403	51.157	43.050	27.594	1.00	53.06	
ATOM	1900	C	GLU	403	56.083	42.237	29.151	1.00	32.03	
ATOM	1901	O	GLU	403	55.627	41.304	29.816	1.00	32.58	
ATOM	1902	N	VAL	404	56.955	42.078	28.159	0.50	31.51	ALTA
ATOM	1903	CA	VAL	404	57.450	40.765	27.739	0.50	30.96	ALTA
ATOM	1904	CB	VAL	404	58.108	40.849	26.333	0.50	30.32	ALTA
ATOM	1905	CG1	VAL	404	58.616	39.489	25.889	0.50	28.72	ALTA
ATOM	1906	CG2	VAL	404	57.115	41.388	25.328	0.50	31.67	ALTA
ATOM	1907	C	VAL	404	58.465	40.149	28.696	0.50	30.45	ALTA
ATOM	1908	O	VAL	404	58.549	38.926	28.822	0.50	30.10	ALTA
ATOM	1909	N	PHE	405	59.224	41.002	29.369	1.00	30.16	
ATOM	1910	CA	PHE	405	60.266	40.549	30.263	1.00	30.65	
ATOM	1911	CB	PHE	405	61.577	41.221	29.863	1.00	28.92	
ATOM	1912	CG	PHE	405	62.062	40.834	28.493	1.00	26.31	
ATOM	1913	CD1	PHE	405	62.342	41.804	27.543	1.00	25.72	
ATOM	1914	CD2	PHE	405	62.269	39.500	28.166	1.00	25.92	
ATOM	1915	CE1	PHE	405	62.827	41.456	26.278	1.00	26.78	
ATOM	1916	CE2	PHE	405	62.752	39.139	26.910	1.00	25.39	
ATOM	1917	CZ	PHE	405	63.034	40.122	25.962	1.00	24.39	
ATOM	1918	C	PHE	405	60.011	40.674	31.771	1.00	32.10	
ATOM	1919	O	PHE	405	60.903	40.237	32.533	1.00	33.88	
ATOM	1920	OXT	PHE	405	58.936	41.169	32.188	1.00	34.95	
ATOM	1	O1	HOH	501	67.542	37.066	11.311	1.00	26.83	
ATOM	3	O1	HOH	502	68.713	41.227	12.821	1.00	23.42	
ATOM	2	O1	HOH	503	64.446	40.325	12.123	1.00	22.84	
ATOM	4	O1	HOH	504	62.236	39.752	15.941	1.00	17.97	
ATOM	5	O1	HOH	505	48.732	20.137	5.515	1.00	50.48	
ATOM	6	O1	HOH	506	47.365	21.522	3.716	1.00	53.40	
ATOM	7	O1	HOH	507	50.211	23.203	7.900	1.00	32.6	

ATOM	12	O1	HOH	512	56.201	16.223	12.164	1.00	18.50
ATOM	13	O1	HOH	513	56.653	12.298	10.528	1.00	27.71
ATOM	14	O1	HOH	514	58.661	10.694	9.014	1.00	46.73
ATOM	15	O1	HOH	515	62.950	10.692	11.952	1.00	43.05
ATOM	16	O1	HOH	516	66.411	11.552	10.897	1.00	37.36
ATOM	17	O1	HOH	517	68.949	13.188	12.029	1.00	39.28
ATOM	18	O1	HOH	518	71.997	15.171	8.362	1.00	49.69
ATOM	19	O1	HOH	519	71.946	17.928	6.743	1.00	24.50
ATOM	20	O1	HOH	520	75.117	15.684	9.377	1.00	35.98
ATOM	21	O1	HOH	521	76.677	12.815	10.294	1.00	49.33
ATOM	22	O1	HOH	522	81.421	15.415	15.139	1.00	46.74
ATOM	23	O1	HOH	523	78.784	21.696	17.564	1.00	49.01
ATOM	24	O1	HOH	524	79.954	24.822	17.152	1.00	42.91
ATOM	25	O1	HOH	525	82.199	30.253	18.821	1.00	40.27
ATOM	26	O1	HOH	526	82.862	33.444	21.988	1.00	46.81
ATOM	27	O1	HOH	527	76.608	30.793	23.452	1.00	46.22
ATOM	28	O1	HOH	528	74.726	30.483	25.469	1.00	43.76
ATOM	29	O1	HOH	529	77.059	28.762	20.900	1.00	33.67
ATOM	30	O1	HOH	530	75.935	33.279	12.269	1.00	25.26
ATOM	31	O1	HOH	531	77.402	34.447	10.087	1.00	37.04
ATOM	32	O1	HOH	532	74.054	29.941	9.998	1.00	26.86
ATOM	33	O1	HOH	533	69.544	32.658	7.572	1.00	40.34
ATOM	34	O1	HOH	534	66.709	33.618	8.477	1.00	20.63
ATOM	35	O1	HOH	535	68.073	35.828	8.931	1.00	23.99
ATOM	36	O1	HOH	536	61.865	45.643	14.011	1.00	40.43
ATOM	37	O1	HOH	537	63.662	46.881	15.670	1.00	28.04
ATOM	38	O1	HOH	538	63.391	49.310	13.883	1.00	39.59
ATOM	39	O1	HOH	539	63.491	50.570	10.631	1.00	52.34
ATOM	40	O1	HOH	540	64.592	46.849	10.299	1.00	26.63
ATOM	41	O1	HOH	541	55.575	41.632	10.980	1.00	38.06
ATOM	42	O1	HOH	542	51.631	42.062	17.343	1.00	45.99
ATOM	43	O1	HOH	543	52.755	43.156	20.209	1.00	34.17
ATOM	44	O1	HOH	544	57.061	49.627	24.004	1.00	24.09
ATOM	45	O1	HOH	545	61.040	50.561	21.351	1.00	30.91
ATOM	46	O1	HOH	546	68.533	53.616	18.390	1.00	30.91
ATOM	47	O1	HOH	547	63.371	58.813	29.014	1.00	59.25
ATOM	48	O1	HOH	548	57.934	52.905	31.175	1.00	40.12
ATOM	49	O1	HOH	549	62.364	50.496	37.543	1.00	52.28
ATOM	50	O1	HOH	550	62.256	49.704	40.891	1.00	54.18
ATOM	51	O1	HOH	551	61.994	46.430	40.384	1.00	43.84
ATOM	52	O1	HOH	552	63.675	44.459	39.268	1.00	44.73
ATOM	53	O1	HOH	553	58.405	43.920	33.936	1.00	42.88
ATOM	54	O1	HOH	554	62.863	39.071	34.046	1.00	45.07
ATOM	55	O1	HOH	555	64.426	36.925	28.676	1.00	25.36
ATOM	56	O1	HOH	556	62.375	35.807	26.610	1.00	21.14
ATOM	57	O1	HOH	557	63.684	33.760	25.609	1.00	33.03
ATOM	58	O1	HOH	558	61.542	29.906	24.568	1.00	57.37

ATOM	59	O1	HOH	559	62.353	27.540	24.855	1.00	39.63
ATOM	60	O1	HOH	560	62.814	28.785	27.536	1.00	58.40
ATOM	61	O1	HOH	561	65.531	30.642	28.821	1.00	54.44
ATOM	62	O1	HOH	562	63.423	24.645	32.964	1.00	50.75
ATOM	63	O1	HOH	563	64.697	21.149	28.711	1.00	51.41
ATOM	64	O1	HOH	564	67.100	23.370	26.900	1.00	52.36
ATOM	65	O1	HOH	565	65.582	20.422	23.303	1.00	40.32
ATOM	66	O1	HOH	566	61.577	18.167	23.386	1.00	65.08
ATOM	67	O1	HOH	567	61.022	22.649	25.573	1.00	48.85
ATOM	68	O1	HOH	568	57.919	21.446	25.147	1.00	43.39
ATOM	69	O1	HOH	569	59.435	20.179	28.543	1.00	51.41
ATOM	70	O1	HOH	570	53.860	23.216	30.984	1.00	50.28
ATOM	71	O1	HOH	571	52.825	24.880	32.696	1.00	43.96
ATOM	72	O1	HOH	572	48.228	29.683	30.486	1.00	44.51
ATOM	73	O1	HOH	573	48.925	34.467	30.521	1.00	36.28
ATOM	74	O1	HOH	574	50.766	40.547	29.178	1.00	51.45
ATOM	75	O1	HOH	575	57.058	32.490	30.420	1.00	31.03
ATOM	76	O1	HOH	576	58.075	29.544	24.664	1.00	19.54
ATOM	77	O1	HOH	577	47.451	19.292	28.703	1.00	33.04
ATOM	78	O1	HOH	578	53.120	15.471	17.478	1.00	35.68
ATOM	79	O1	HOH	579	55.101	14.146	16.095	1.00	50.46
ATOM	80	O1	HOH	580	53.726	14.016	9.059	1.00	41.44
ATOM	81	O1	HOH	581	57.223	13.820	1.435	1.00	48.31
ATOM	82	O1	HOH	582	61.169	15.688	0.210	1.00	17.60
ATOM	83	O1	HOH	583	67.411	16.019	-0.314	1.00	23.93
ATOM	84	O1	HOH	584	67.033	17.221	-2.796	1.00	26.21
ATOM	85	O1	HOH	585	69.893	19.520	-1.582	1.00	59.67
ATOM	86	O1	HOH	586	68.489	22.464	0.350	1.00	37.85
ATOM	87	O1	HOH	587	65.794	23.354	0.823	1.00	27.38
ATOM	88	O1	HOH	588	67.550	26.810	0.937	1.00	37.18
ATOM	89	O1	HOH	589	64.646	28.208	3.323	1.00	36.74
ATOM	90	O1	HOH	590	67.215	31.103	3.174	1.00	30.29
ATOM	91	O1	HOH	591	64.164	35.667	6.220	1.00	39.72
ATOM	92	O1	HOH	592	62.810	37.518	4.836	1.00	48.48
ATOM	93	O1	HOH	593	68.105	36.898	6.110	1.00	58.00
ATOM	94	O1	HOH	594	57.390	37.485	2.631	1.00	37.29
ATOM	95	O1	HOH	595	53.088	36.068	3.949	1.00	50.10
ATOM	96	O1	HOH	596	52.974	34.676	6.758	1.00	42.52
ATOM	97	O1	HOH	597	58.581	31.465	2.076	1.00	32.18
ATOM	98	O1	HOH	598	52.786	23.277	1.357	1.00	28.98
ATOM	99	O1	HOH	599	47.501	26.551	7.672	1.00	47.83
ATOM	100	O1	HOH	600	46.411	35.754	14.049	1.00	53.46
ATOM	101	O1	HOH	601	63.514	14.944	15.842	1.00	55.02
ATOM	102	O1	HOH	602	67.943	11.792	3.438	1.00	61.21
ATOM	103	O1	HOH	603	62.232	9.378	3.311	1.00	35.65
ATOM	104	O1	HOH	604	76.734	22.468	5.		

ATOM	106	O1	HOH	606	82.807	43.437	17.940	1.00	39.28
ATOM	107	O1	HOH	607	83.882	45.673	20.638	1.00	41.64
ATOM	108	O1	HOH	608	80.215	41.021	23.441	1.00	43.16
ATOM	109	O1	HOH	609	79.459	46.296	31.165	1.00	32.40
ATOM	110	O1	HOH	610	81.880	47.681	33.923	1.00	46.96
ATOM	111	O1	HOH	611	75.594	46.142	30.384	1.00	28.64
ATOM	112	O1	HOH	612	77.118	40.568	32.575	1.00	34.21
ATOM	113	O1	HOH	613	73.563	41.750	36.926	1.00	26.07
ATOM	114	O1	HOH	614	75.955	56.565	28.863	1.00	46.31
ATOM	115	O1	HOH	615	79.915	59.136	15.809	1.00	50.81
ATOM	116	O1	HOH	616	77.390	52.542	8.816	1.00	34.34
ATOM	117	O1	HOH	617	72.726	25.005	29.671	1.00	62.84
ATOM	2038	C	ACY	701	52.664	40.106	24.800	1.00	46.39
ATOM	2039	O	ACY	701	53.721	39.649	24.298	1.00	47.12
ATOM	2040	OXT	ACY	701	51.652	40.521	24.172	1.00	46.96
ATOM	2041	CH3	ACY	701	52.600	40.162	26.329	1.00	45.99
ATOM	2050	C1	T3	1	66.961	42.243	18.491	1.00	22.34
ATOM	2051	C2	T3	1	68.748	43.593	23.015	1.00	21.84
ATOM	2052	C3	T3	1	66.873	43.557	18.970	1.00	23.43
ATOM	2053	C4	T3	1	69.252	44.540	23.871	1.00	22.31
ATOM	2054	C5	T3	1	67.638	43.989	20.011	1.00	24.83
ATOM	2055	C6	T3	1	68.851	44.553	25.178	1.00	25.16
ATOM	2056	C7	T3	1	68.541	43.108	20.632	1.00	24.65
ATOM	2057	C8	T3	1	67.895	43.567	25.639	1.00	21.93
ATOM	2058	C9	T3	1	68.665	41.792	20.183	1.00	25.09
ATOM	2059	C10	T3	1	67.427	42.654	24.733	1.00	23.66
ATOM	2060	C11	T3	1	67.878	41.380	19.117	1.00	23.12
ATOM	2061	C12	T3	1	67.829	42.624	23.384	1.00	19.67
ATOM	2062	C13	T3	1	66.055	41.788	17.371	1.00	18.97
ATOM	2063	C15	T3	1	66.721	40.956	16.295	1.00	19.32
ATOM	2064	C17	T3	1	65.901	40.829	15.051	1.00	19.02
ATOM	2065	I1	T3	1	67.393	45.986	20.621	1.00	25.29
ATOM	2066	I2	T3	1	69.483	46.066	26.432	1.00	26.49
ATOM	2067	I3	T3	1	70.019	40.450	20.975	1.00	25.67
ATOM	2068	N1	T3	1	68.131	41.337	16.037	1.00	15.12
ATOM	2069	O1	T3	1	67.542	43.587	26.966	1.00	21.79
ATOM	2070	O2	T3	1	69.259	43.600	21.682	1.00	22.05
ATOM	2071	O3	T3	1	66.504	40.852	13.963	1.00	20.38
ATOM	2072	O4	T3	1	64.675	40.731	15.192	1.00	20.16
END									



## APPENDIX 7

### TRBTRIAC.PDB

REMARK TR-beta Triac Full length numbering  
 REMARK refinement resolution: 100 - 2.9 A r= 0.273258 free\_r= 0.333794  
 REMARK wa= 5.78307  
 REMARK target= mlf cycles= 1 steps= 25  
 REMARK a= 68.72 b= 68.72 c= 130.092 alpha= 90 beta= 90 gamma= 120  
 REMARK ncs= none  
 REMARK initial B-factor correction: "none"  
 REMARK ALA 199 to ALA 201 from His-tag  
 REMARK  
 REMARK Four cacodylate-modified cysteines (CYA)  
 REMARK Cys294, Cys298, Cys388, Cys434  
 REMARK cacodylate modeled as single arsenic atom  
 REMARK  
 REMARK side chain of certain residues modeled as ALA due to poor density;  
 REMARK however, residue name reflects true residue for clarity  
 REMARK  
 REMARK amino acid sequence confirmed,  
 REMARK differing from that reported by Weinberger et. al.  
 REMARK in the following codons:  
 REMARK 243 Pro - Arg  
 REMARK 337 Ile - Thr  
 REMARK 451 Leu - Phe  
 REMARK as reported by Sakurai et. al.  
 REMARK note also correction of initiation codon,  
 REMARK yielding a polypeptide of 461 amino acids

JRNL AUTH A.SAKURAI,A.NAKAI,L.J.DEGROOT  
 JRNL TITL STRUCTURAL ANALYSIS OF HUMAN THYROID HORMONE RECEPTOR  
 JRNL TITL2 BETA GENE  
 JRNL REF MOL.CELL.ENDO. V.71 1990  
 JRNL AUTH C.WEINBERGER, C.C.THOMPSON,R.LEBO,D.J.GRUOL,R.M.EVANS  
 JRNL TITL THE C-ERB-A GENE ENCODES A THYROID HORMONE RECEPTOR  
 JRNL REF NATURE V.324 6098 1986

ATOM	1	CB	ALA	199	31.247	28.289	43.613	1.00	71.30	PROT
ATOM	2	C	ALA	199	32.916	26.485	44.170	1.00	68.99	PROT
ATOM	3	O	ALA	199	33.485	25.410	43.976	1.00	63.84	PROT
ATOM	4	N	ALA	199	30.462	25.993	44.096	1.00	75.00	PROT
ATOM	5	CA	ALA	199	31.571	26.795	43.497	1.00	73.24	PROT
ATOM	6	N	ALA	200	33.419	27.432	44.958	1.00	73.81	PROT
ATOM	7	CA	ALA	200	34.686	27.251	45.658	1.00	67.87	PROT
ATOM	8	CB	ALA	200	35.182	28.583	46.203	1.00	62.83	PROT
ATOM	9	C	ALA	200	34.539	26.239	46.791	1.00	63.23	PROT



ATOM	10	O	ALA	200	35.486	25.986	47.534	1.00	59.14	PROT
ATOM	11	N	ALA	201	33.345	25.670	46.932	1.00	56.98	PROT
ATOM	12	CA	ALA	201	33.117	24.664	47.957	1.00	51.46	PROT
ATOM	13	CB	ALA	201	31.776	23.992	47.744	1.00	40.35	PROT
ATOM	14	C	ALA	201	34.248	23.662	47.762	1.00	53.15	PROT
ATOM	15	O -	ALA	201	34.624	22.938	48.679	1.00	54.90	PROT
ATOM	16	N	GLU	202	34.789	23.645	46.546	1.00	44.13	PROT
ATOM	17	CA	GLU	202	35.891	22.767	46.190	1.00	37.47	PROT
ATOM	18	CB	GLU	202	36.086	22.760	44.671	1.00	37.74	PROT
ATOM	19	CG	GLU	202	37.060	21.702	44.173	1.00	57.14	PROT
ATOM	20	CD	GLU	202	36.457	20.303	44.140	1.00	61.74	PROT
ATOM	21	OE1	GLU	202	35.211	20.175	44.133	1.00	63.81	PROT
ATOM	22	OE2	GLU	202	37.236	19.327	44.115	1.00	65.54	PROT
ATOM	23	C	GLU	202	37.156	23.266	46.878	1.00	35.54	PROT
ATOM	24	O	GLU	202	37.874	22.492	47.510	1.00	32.70	PROT
ATOM	25	N	GLU	203	37.415	24.566	46.755	1.00	31.79	PROT
ATOM	26	CA	GLU	203	38.588	25.188	47.366	1.00	33.63	PROT
ATOM	27	CB	GLU	203	38.603	26.683	47.079	1.00	28.28	PROT
ATOM	28	C	GLU	203	38.588	24.948	48.869	1.00	33.86	PROT
ATOM	29	O	GLU	203	39.644	24.818	49.485	1.00	33.10	PROT
ATOM	30	N	LEU	204	37.393	24.898	49.451	1.00	34.15	PROT
ATOM	31	CA	LEU	204	37.244	24.650	50.876	1.00	33.22	PROT
ATOM	32	CB	LEU	204	35.853	25.081	51.353	1.00	30.47	PROT
ATOM	33	CG	LEU	204	35.567	25.083	52.862	1.00	23.17	PROT
ATOM	34	CD1	LEU	204	35.904	26.439	53.443	1.00	5.41	PROT
ATOM	35	CD2	LEU	204	34.106	24.748	53.111	1.00	12.70	PROT
ATOM	36	C	LEU	204	37.424	23.156	51.100	1.00	40.17	PROT
ATOM	37	O	LEU	204	38.219	22.736	51.951	1.00	45.33	PROT
ATOM	38	N	GLN	205	36.682	22.360	50.329	1.00	43.86	PROT
ATOM	39	CA	GLN	205	36.754	20.899	50.415	1.00	43.96	PROT
ATOM	40	CB	GLN	205	36.089	20.261	49.184	1.00	45.56	PROT
ATOM	41	CG	GLN	205	34.562	20.195	49.245	1.00	42.39	PROT
ATOM	42	CD	GLN	205	34.022	18.775	49.159	1.00	46.79	PROT
ATOM	43	OE1	GLN	205	33.258	18.444	48.252	1.00	38.84	PROT
ATOM	44	NE2	GLN	205	34.412	17.932	50.109	1.00	37.95	PROT
ATOM	45	C	GLN	205	38.224	20.482	50.483	1.00	42.39	PROT
ATOM	46	O	GLN	205	38.630	19.702	51.355	1.00	36.27	PROT
ATOM	47	N	LYS	206	39.014	21.015	49.553	1.00	42.37	PROT
ATOM	48	CA	LYS	206	40.440	20.729	49.505	1.00	44.40	PROT
ATOM	49	CB	LYS	206	41.110	21.531	48.385	1.00	38.73	PROT
ATOM	50	C	LYS	206	41.024	21.118	50.853	1.00	42.36	PROT
ATOM	51	O	LYS	206	41.550	20.271	51.570	1.00	46.93	PROT
ATOM	52	N	SER	207	40.					

ATOM	56	C	SER	207	41.254	21.958	53.614	1.00	29.20	PROT
ATOM	57	O	SER	207	42.223	21.623	54.293	1.00	31.01	PROT
ATOM	58	N	ILE	208	40.028	21.504	53.841	1.00	22.55	PROT
ATOM	59	CA	ILE	208	39.777	20.568	54.928	1.00	27.93	PROT
ATOM	60	CB	ILE	208	38.267	20.216	55.027	1.00	39.85	PROT
ATOM	61	CG2	ILE	208	38.062	18.895	55.769	1.00	32.13	PROT
ATOM	62	CG1	ILE	208	37.528	21.340	55.753	1.00	37.63	PROT
ATOM	63	CD1	ILE	208	36.788	22.296	54.827	1.00	41.47	PROT
ATOM	64	C	ILE	208	40.591	19.291	54.725	1.00	29.61	PROT
ATOM	65	O	ILE	208	40.905	18.580	55.679	1.00	40.00	PROT
ATOM	66	N	GLY	209	40.928	19.002	53.475	1.00	35.05	PROT
ATOM	67	CA	GLY	209	41.698	17.809	53.181	1.00	31.94	PROT
ATOM	68	C	GLY	209	40.826	16.695	52.643	1.00	28.66	PROT
ATOM	69	O	GLY	209	41.257	15.553	52.532	1.00	19.46	PROT
ATOM	70	N	HIS	210	39.586	17.021	52.313	1.00	20.47	PROT
ATOM	71	CA	HIS	210	38.684	16.018	51.774	1.00	26.99	PROT
ATOM	72	CB	HIS	210	37.240	16.451	52.012	1.00	37.16	PROT
ATOM	73	C	HIS	210	38.959	15.806	50.266	1.00	27.75	PROT
ATOM	74	O	HIS	210	39.328	16.741	49.550	1.00	34.08	PROT
ATOM	75	N	LYS	211	38.807	14.566	49.805	1.00	16.50	PROT
ATOM	76	CA	LYS	211	39.019	14.206	48.403	1.00	5.57	PROT
ATOM	77	CB	LYS	211	39.932	12.981	48.295	1.00	5.67	PROT
ATOM	78	CG	LYS	211	41.370	13.208	48.742	1.00	7.30	PROT
ATOM	79	CD	LYS	211	41.873	14.594	48.347	1.00	14.34	PROT
ATOM	80	CE	LYS	211	43.339	14.556	47.897	1.00	29.48	PROT
ATOM	81	NZ	LYS	211	43.777	15.851	47.262	1.00	33.43	PROT
ATOM	82	C	LYS	211	37.642	13.861	47.876	1.00	2.73	PROT
ATOM	83	O	LYS	211	37.176	12.741	48.039	1.00	6.57	PROT
ATOM	84	N	PRO	212	36.983	14.813	47.208	1.00	2.00	PROT
ATOM	85	CD	PRO	212	37.472	16.156	46.846	1.00	10.43	PROT
ATOM	86	CA	PRO	212	35.642	14.542	46.689	1.00	2.05	PROT
ATOM	87	CB	PRO	212	35.088	15.928	46.341	1.00	10.09	PROT
ATOM	88	CG	PRO	212	36.240	16.888	46.422	1.00	8.43	PROT
ATOM	89	C	PRO	212	35.523	13.578	45.520	1.00	2.00	PROT
ATOM	90	O	PRO	212	36.344	13.554	44.611	1.00	6.04	PROT
ATOM	91	N	GLU	213	34.476	12.773	45.577	1.00	2.68	PROT
ATOM	92	CA	GLU	213	34.181	11.817	44.542	1.00	6.81	PROT
ATOM	93	CB	GLU	213	33.539	10.594	45.173	1.00	7.20	PROT
ATOM	94	CG	GLU	213	34.222	10.232	46.462	1.00	15.33	PROT
ATOM	95	CD	GLU	213	34.293	8.743	46.689	1.00	21.36	PROT
ATOM	96	OE1	GLU	213	33.334	8.051	46.290	1.00	29.32	PROT
ATOM	97	OE2	GLU	213	35.301	8.265	47.268	1.00	28.50	PROT
ATOM	98	C	GLU	213	33.229	12.543	43.584	1		

ATOM	102	CA	PRO	214	32.145	12.536	41.322	1.00	23.38	PROT
ATOM	103	CB	PRO	214	32.180	11.476	40.232	1.00	18.01	PROT
ATOM	104	CG	PRO	214	33.376	10.665	40.514	1.00	27.50	PROT
ATOM	105	C	PRO	214	30.715	12.828	41.734	1.00	25.02	PROT
ATOM	106	O	PRO	214	30.069	11.986	42.355	1.00	31.17	PROT
ATOM	107	N-	THR	215	30.211	14.009	41.377	1.00	19.56	PROT
ATOM	108	CA	THR	215	28.830	14.352	41.714	1.00	24.48	PROT
ATOM	109	CB	THR	215	28.535	15.841	41.522	1.00	27.13	PROT
ATOM	110	OG1	THR	215	27.939	16.038	40.234	1.00	40.19	PROT
ATOM	111	CG2	THR	215	29.805	16.659	41.640	1.00	30.81	PROT
ATOM	112	C	THR	215	27.899	13.562	40.805	1.00	22.14	PROT
ATOM	113	O	THR	215	28.357	12.905	39.883	1.00	27.52	PROT
ATOM	114	N	ASP	216	26.599	13.617	41.072	1.00	35.65	PROT
ATOM	115	CA	ASP	216	25.631	12.890	40.258	1.00	41.16	PROT
ATOM	116	CB	ASP	216	24.219	13.091	40.810	1.00	38.17	PROT
ATOM	117	C	ASP	216	25.714	13.370	38.810	1.00	40.44	PROT
ATOM	118	O	ASP	216	25.683	12.569	37.874	1.00	38.26	PROT
ATOM	119	N	GLU	217	25.832	14.682	38.635	1.00	40.14	PROT
ATOM	120	CA	GLU	217	25.932	15.275	37.305	1.00	38.89	PROT
ATOM	121	CB	GLU	217	25.883	16.796	37.413	1.00	29.95	PROT
ATOM	122	C	GLU	217	27.231	14.829	36.619	1.00	39.44	PROT
ATOM	123	O	GLU	217	27.245	14.525	35.425	1.00	40.08	PROT
ATOM	124	N	GLU	218	28.319	14.794	37.384	1.00	34.92	PROT
ATOM	125	CA	GLU	218	29.615	14.370	36.871	1.00	23.70	PROT
ATOM	126	CB	GLU	218	30.698	14.606	37.924	1.00	18.47	PROT
ATOM	127	CG	GLU	218	30.990	16.067	38.198	1.00	15.66	PROT
ATOM	128	CD	GLU	218	32.085	16.264	39.231	1.00	26.88	PROT
ATOM	129	OE1	GLU	218	32.164	15.458	40.191	1.00	25.07	PROT
ATOM	130	OE2	GLU	218	32.864	17.232	39.078	1.00	33.79	PROT
ATOM	131	C	GLU	218	29.589	12.892	36.491	1.00	21.05	PROT
ATOM	132	O	GLU	218	30.182	12.490	35.495	1.00	24.30	PROT
ATOM	133	N	TRP	219	28.907	12.080	37.288	1.00	13.98	PROT
ATOM	134	CA	TRP	219	28.829	10.660	37.000	1.00	17.30	PROT
ATOM	135	CB	TRP	219	28.052	9.921	38.089	1.00	16.27	PROT
ATOM	136	CG	TRP	219	28.890	9.520	39.277	1.00	31.14	PROT
ATOM	137	CD2	TRP	219	29.984	8.585	39.296	1.00	36.40	PROT
ATOM	138	CE2	TRP	219	30.476	8.547	40.621	1.00	29.24	PROT
ATOM	139	CE3	TRP	219	30.595	7.781	38.323	1.00	41.61	PROT
ATOM	140	CD1	TRP	219	28.771	9.988	40.551	1.00	28.69	PROT
ATOM	141	NE1	TRP	219	29.718	9.411	41.362	1.00	35.01	PROT
ATOM	142	CZ2	TRP	219	31.552	7.737	41.004	1.00	30.89	PROT
ATOM	143	CZ3	TRP	219	31.673	6.969	38.707	1.00	45.72	PROT
ATOM										

ATOM	148	CA	GLU	220	26.400	11.323	34.159	1.00	33.95	PROT
ATOM	149	CB	GLU	220	25.237	12.318	34.201	1.00	22.17	PROT
ATOM	150	C	GLU	220	27.356	11.658	33.013	1.00	34.66	PROT
ATOM	151	O	GLU	220	27.233	11.134	31.900	1.00	43.86	PROT
ATOM	152	N	LEU	221	28.320	12.528	33.297	1.00	22.60	PROT
ATOM	153	CA	LEU	221	29.305	12.926	32.304	1.00	17.18	PROT
ATOM	154	CB	LEU	221	29.995	14.219	32.743	1.00	11.03	PROT
ATOM	155	CG	LEU	221	31.078	14.824	31.850	1.00	5.17	PROT
ATOM	156	CD1	LEU	221	30.756	14.569	30.415	1.00	6.41	PROT
ATOM	157	CD2	LEU	221	31.181	16.305	32.092	1.00	10.65	PROT
ATOM	158	C	LEU	221	30.344	11.817	32.122	1.00	22.25	PROT
ATOM	159	O	LEU	221	30.759	11.521	31.002	1.00	18.99	PROT
ATOM	160	N	ILE	222	30.754	11.198	33.228	1.00	20.74	PROT
ATOM	161	CA	ILE	222	31.744	10.136	33.177	1.00	12.88	PROT
ATOM	162	CB	ILE	222	32.115	9.662	34.587	1.00	12.96	PROT
ATOM	163	CG2	ILE	222	33.030	8.468	34.515	1.00	2.00	PROT
ATOM	164	CG1	ILE	222	32.811	10.796	35.332	1.00	16.50	PROT
ATOM	165	CD1	ILE	222	33.625	10.351	36.511	1.00	15.90	PROT
ATOM	166	C	ILE	222	31.241	8.958	32.363	1.00	17.72	PROT
ATOM	167	O	ILE	222	32.001	8.363	31.594	1.00	16.59	PROT
ATOM	168	N	LYS	223	29.966	8.618	32.530	1.00	33.88	PROT
ATOM	169	CA	LYS	223	29.371	7.503	31.795	1.00	39.02	PROT
ATOM	170	CB	LYS	223	27.908	7.307	32.224	1.00	40.29	PROT
ATOM	171	C	LYS	223	29.444	7.779	30.293	1.00	39.14	PROT
ATOM	172	O	LYS	223	29.949	6.963	29.517	1.00	32.99	PROT
ATOM	173	N	THR	224	28.936	8.942	29.897	1.00	27.19	PROT
ATOM	174	CA	THR	224	28.929	9.363	28.498	1.00	25.75	PROT
ATOM	175	CB	THR	224	28.440	10.817	28.407	1.00	22.51	PROT
ATOM	176	OG1	THR	224	27.018	10.837	28.568	1.00	35.46	PROT
ATOM	177	CG2	THR	224	28.799	11.436	27.083	1.00	15.53	PROT
ATOM	178	C	THR	224	30.307	9.235	27.833	1.00	22.31	PROT
ATOM	179	O	THR	224	30.480	8.517	26.843	1.00	27.13	PROT
ATOM	180	N	VAL	225	31.287	9.936	28.386	1.00	17.87	PROT
ATOM	181	CA	VAL	225	32.635	9.906	27.854	1.00	17.07	PROT
ATOM	182	CB	VAL	225	33.559	10.759	28.720	1.00	16.86	PROT
ATOM	183	CG1	VAL	225	34.845	11.064	27.973	1.00	26.54	PROT
ATOM	184	CG2	VAL	225	32.854	12.057	29.075	1.00	24.46	PROT
ATOM	185	C	VAL	225	33.169	8.486	27.793	1.00	16.11	PROT
ATOM	186	O	VAL	225	33.683	8.042	26.763	1.00	12.75	PROT
ATOM	187	N	THR	226	33.040	7.769	28.900	1.00	12.23	PROT
ATOM	188	CA	THR	226	33.520	6.400	28.951	1.00	12.34	PROT
ATOM	189	CB	THR	226	33.175	5.747	30.271	1.00	17.01	PROT
ATOM	190	OG1	THR	226</						



ATOM	194	N	GLU	227	31.582	5.588	27.758	1.00	22.90	PROT
ATOM	195	CA	GLU	227	30.886	4.849	26.714	1.00	22.63	PROT
ATOM	196	CB	GLU	227	29.417	5.248	26.678	1.00	20.14	PROT
ATOM	197	C	GLU	227	31.556	5.173	25.386	1.00	21.74	PROT
ATOM	198	O	GLU	227	32.057	4.283	24.700	1.00	24.42	PROT
ATOM	199	N	ALA	228	31.590	6.460	25.050	1.00	13.26	PROT
ATOM	200	CA	ALA	228	32.196	6.928	23.800	1.00	22.76	PROT
ATOM	201	CB	ALA	228	32.267	8.450	23.785	1.00	22.50	PROT
ATOM	202	C	ALA	228	33.584	6.358	23.538	1.00	19.19	PROT
ATOM	203	O	ALA	228	33.913	6.003	22.408	1.00	17.19	PROT
ATOM	204	N	HIS	229	34.408	6.290	24.573	1.00	20.11	PROT
ATOM	205	CA	HIS	229	35.741	5.756	24.389	1.00	18.68	PROT
ATOM	206	CB	HIS	229	36.537	5.819	25.686	1.00	10.37	PROT
ATOM	207	CG	HIS	229	37.894	5.201	25.586	1.00	2.00	PROT
ATOM	208	CD2	HIS	229	38.524	4.299	26.376	1.00	7.61	PROT
ATOM	209	ND1	HIS	229	38.780	5.517	24.582	1.00	3.78	PROT
ATOM	210	CE1	HIS	229	39.900	4.837	24.758	1.00	15.67	PROT
ATOM	211	NE2	HIS	229	39.771	4.090	25.840	1.00	7.10	PROT
ATOM	212	C	HIS	229	35.637	4.316	23.940	1.00	21.45	PROT
ATOM	213	O	HIS	229	36.127	3.950	22.866	1.00	22.42	PROT
ATOM	214	N	VAL	230	34.983	3.505	24.762	1.00	21.64	PROT
ATOM	215	CA	VAL	230	34.827	2.086	24.468	1.00	33.80	PROT
ATOM	216	CB	VAL	230	33.960	1.388	25.528	1.00	33.11	PROT
ATOM	217	CG1	VAL	230	34.251	-0.106	25.515	1.00	33.80	PROT
ATOM	218	CG2	VAL	230	34.228	1.985	26.896	1.00	26.54	PROT
ATOM	219	C	VAL	230	34.224	1.781	23.100	1.00	33.12	PROT
ATOM	220	O	VAL	230	34.703	0.897	22.385	1.00	40.80	PROT
ATOM	221	N	ALA	231	33.170	2.507	22.746	1.00	36.22	PROT
ATOM	222	CA	ALA	231	32.497	2.298	21.471	1.00	36.24	PROT
ATOM	223	CB	ALA	231	31.318	3.255	21.343	1.00	18.90	PROT
ATOM	224	C	ALA	231	33.445	2.501	20.303	1.00	37.54	PROT
ATOM	225	O	ALA	231	33.342	1.816	19.285	1.00	35.93	PROT
ATOM	226	N	THR	232	34.380	3.434	20.474	1.00	23.74	PROT
ATOM	227	CA	THR	232	35.329	3.789	19.432	1.00	15.54	PROT
ATOM	228	CB	THR	232	35.335	5.321	19.238	1.00	9.70	PROT
ATOM	229	OG1	THR	232	35.733	5.949	20.460	1.00	16.73	PROT
ATOM	230	CG2	THR	232	33.942	5.828	18.891	1.00	2.00	PROT
ATOM	231	C	THR	232	36.758	3.309	19.670	1.00	19.86	PROT
ATOM	232	O	THR	232	37.695	3.854	19.094	1.00	15.31	PROT
ATOM	233	N	ASN	233	36.938	2.305	20.523	1.00	28.26	PROT
ATOM	234	CA	ASN	233	38.280	1.771	20.772	1.00	39.32	PROT
ATOM	235	CB	ASN	233	38.435	1.343	22.234	1.00	47.14	PROT
ATOM	236	CG	ASN	233	39.804	1.689	22.801	1.00		



ATOM	240	O	ASN	233	38.338	0.693	18.625	1.00	65.36	PROT
ATOM	241	N	ALA	234	38.877	-0.577	20.388	1.00	57.89	PROT
ATOM	242	CA	ALA	234	39.090	-1.752	19.552	1.00	57.22	PROT
ATOM	243	CB	ALA	234	40.372	-1.595	18.754	1.00	48.03	PROT
ATOM	244	C	ALA	234	39.141	-3.027	20.384	1.00	62.42	PROT
ATOM	245	O.	ALA	234	38.471	-3.073	21.440	1.00	56.93	PROT
ATOM	246	OT	ALA	234	39.853	-3.968	19.965	1.00	76.16	PROT
ATOM	247	N	TRP	239	41.987	-7.449	22.970	1.00	58.82	PROT
ATOM	248	CA	TRP	239	43.077	-6.886	22.154	1.00	51.37	PROT
ATOM	249	CB	TRP	239	43.325	-5.406	22.534	1.00	45.12	PROT
ATOM	250	CG	TRP	239	44.193	-5.170	23.760	1.00	43.09	PROT
ATOM	251	CD2	TRP	239	45.617	-5.037	23.793	1.00	32.36	PROT
ATOM	252	CE2	TRP	239	45.990	-4.872	25.142	1.00	28.37	PROT
ATOM	253	CE3	TRP	239	46.615	-5.049	22.813	1.00	40.79	PROT
ATOM	254	CD1	TRP	239	43.773	-5.073	25.059	1.00	46.63	PROT
ATOM	255	NE1	TRP	239	44.847	-4.896	25.893	1.00	27.08	PROT
ATOM	256	CZ2	TRP	239	47.315	-4.717	25.535	1.00	35.48	PROT
ATOM	257	CZ3	TRP	239	47.936	-4.896	23.204	1.00	40.18	PROT
ATOM	258	CH2	TRP	239	48.273	-4.733	24.554	1.00	49.93	PROT
ATOM	259	C	TRP	239	44.422	-7.623	22.063	1.00	49.76	PROT
ATOM	260	O	TRP	239	44.944	-7.799	20.962	1.00	48.14	PROT
ATOM	261	N	LYS	240	44.975	-8.048	23.198	1.00	38.92	PROT
ATOM	262	CA	LYS	240	46.263	-8.735	23.232	1.00	37.29	PROT
ATOM	263	CB	LYS	240	46.572	-9.196	24.657	1.00	38.79	PROT
ATOM	264	CG	LYS	240	47.106	-8.099	25.571	1.00	38.43	PROT
ATOM	265	CD	LYS	240	48.307	-8.584	26.370	1.00	35.71	PROT
ATOM	266	CE	LYS	240	48.631	-7.646	27.523	1.00	37.87	PROT
ATOM	267	NZ	LYS	240	49.058	-8.377	28.750	1.00	28.85	PROT
ATOM	268	C	LYS	240	46.404	-9.914	22.269	1.00	42.18	PROT
ATOM	269	O	LYS	240	47.491	-10.132	21.732	1.00	45.89	PROT
ATOM	270	N	GLN	241	45.331	-10.679	22.058	1.00	46.08	PROT
ATOM	271	CA	GLN	241	45.390	-11.816	21.133	1.00	45.02	PROT
ATOM	272	CB	GLN	241	44.575	-13.011	21.638	1.00	46.30	PROT
ATOM	273	CG	GLN	241	44.284	-13.018	23.116	1.00	60.38	PROT
ATOM	274	CD	GLN	241	42.828	-13.312	23.408	1.00	63.76	PROT
ATOM	275	OE1	GLN	241	42.154	-13.988	22.631	1.00	66.34	PROT
ATOM	276	NE2	GLN	241	42.333	-12.801	24.531	1.00	69.18	PROT
ATOM	277	C	GLN	241	44.866	-11.405	19.764	1.00	45.77	PROT
ATOM	278	O	GLN	241	45.107	-12.085	18.765	1.00	51.18	PROT
ATOM	279	N	LYS	242	44.132	-10.300	19.723	1.00	42.04	PROT
ATOM	280	CA	LYS	242	43.613	-9.794	18.464	1.00	48.33	PROT
ATOM	281	CB	LYS	242	42.498	-8.786	18.727	1.00	40.17	PROT
ATOM	282	C								

ATOM	286	CB	ARG	243	48.108	-8.135	19.118	1.00	40.21	PROT
ATOM	287	C	ARG	243	47.795	-9.220	16.892	1.00	45.96	PROT
ATOM	288	O	ARG	243	47.684	-10.443	16.894	1.00	50.22	PROT
ATOM	289	N	LYS	244	48.498	-8.551	15.982	1.00	52.12	PROT
ATOM	290	CA	LYS	244	49.202	-9.202	14.879	1.00	45.30	PROT
ATOM	291	CB	LYS	244	48.466	-8.950	13.558	1.00	48.24	PROT
ATOM	292	CG	LYS	244	47.109	-9.631	13.446	1.00	53.78	PROT
ATOM	293	CD	LYS	244	46.835	-10.078	12.011	1.00	60.50	PROT
ATOM	294	CE	LYS	244	46.038	-9.030	11.241	1.00	61.03	PROT
ATOM	295	NZ	LYS	244	45.455	-7.997	12.146	1.00	55.25	PROT
ATOM	296	C	LYS	244	50.616	-8.641	14.786	1.00	40.33	PROT
ATOM	297	O	LYS	244	50.849	-7.629	14.125	1.00	36.07	PROT
ATOM	298	N	PHE	245	51.556	-9.312	15.445	1.00	27.87	PROT
ATOM	299	CA	PHE	245	52.949	-8.885	15.461	1.00	30.61	PROT
ATOM	300	CB	PHE	245	53.784	-9.887	16.253	1.00	20.28	PROT
ATOM	301	CG	PHE	245	53.454	-9.922	17.713	1.00	37.23	PROT
ATOM	302	CD1	PHE	245	52.636	-10.917	18.234	1.00	40.93	PROT
ATOM	303	CD2	PHE	245	53.958	-8.959	18.577	1.00	41.60	PROT
ATOM	304	CE1	PHE	245	52.326	-10.953	19.594	1.00	42.54	PROT
ATOM	305	CE2	PHE	245	53.652	-8.989	19.936	1.00	45.84	PROT
ATOM	306	CZ	PHE	245	52.835	-9.988	20.443	1.00	33.72	PROT
ATOM	307	C	PHE	245	53.549	-8.693	14.068	1.00	38.75	PROT
ATOM	308	O	PHE	245	53.794	-9.660	13.337	1.00	48.93	PROT
ATOM	309	N	LEU	246	53.789	-7.437	13.704	1.00	41.18	PROT
ATOM	310	CA	LEU	246	54.362	-7.124	12.404	1.00	43.43	PROT
ATOM	311	CB	LEU	246	54.378	-5.612	12.181	1.00	42.78	PROT
ATOM	312	CG	LEU	246	54.535	-5.200	10.718	1.00	49.88	PROT
ATOM	313	CD1	LEU	246	53.528	-4.113	10.365	1.00	40.64	PROT
ATOM	314	CD2	LEU	246	55.966	-4.730	10.485	1.00	48.66	PROT
ATOM	315	C	LEU	246	55.777	-7.692	12.250	1.00	42.60	PROT
ATOM	316	O	LEU	246	56.677	-7.383	13.028	1.00	45.75	PROT
ATOM	317	N	PRO	247	55.977	-8.540	11.233	1.00	50.03	PROT
ATOM	318	CD	PRO	247	54.914	-8.924	10.286	1.00	60.17	PROT
ATOM	319	CA	PRO	247	57.237	-9.199	10.894	1.00	49.90	PROT
ATOM	320	CB	PRO	247	57.181	-9.282	9.369	1.00	59.51	PROT
ATOM	321	CG	PRO	247	55.678	-9.244	9.023	1.00	52.86	PROT
ATOM	322	C	PRO	247	58.499	-8.494	11.392	1.00	48.85	PROT
ATOM	323	O	PRO	247	58.675	-7.295	11.186	1.00	49.28	PROT
ATOM	324	N	GLU	248	59.379	-9.261	12.032	1.00	47.62	PROT
ATOM	325	CA	GLU	248	60.628	-8.733	12.574	1.00	51.41	PROT
ATOM	326	CB	GLU	248	61.266	-9.750	13.522	1.00	44.22	PROT
ATOM	327	C	GLU	248	61.623	-8.354	11.490	1.00	53.28	PROT
ATOM	328	O	GLU	248	62.815	-				

ATOM	332	CG ASP	249	60.928	-9.637	7.739	1.00	54.39	PROT
ATOM	333	OD1 ASP	249	60.578	-10.693	8.310	1.00	57.70	PROT
ATOM	334	OD2 ASP	249	60.264	-9.112	6.819	1.00	45.76	PROT
ATOM	335	C ASP	249	61.539	-6.567	8.437	1.00	54.20	PROT
ATOM	336	O ASP	249	62.119	-6.154	7.429	1.00	55.31	PROT
ATOM	337	N ILE	250	60.469	-5.965	8.954	1.00	46.13	PROT
ATOM	338	CA ILE	250	59.933	-4.735	8.376	1.00	46.12	PROT
ATOM	339	CB ILE	250	58.413	-4.764	8.253	1.00	43.38	PROT
ATOM	340	CG2 ILE	250	57.892	-3.344	8.057	1.00	39.15	PROT
ATOM	341	CG1 ILE	250	58.007	-5.654	7.074	1.00	48.96	PROT
ATOM	342	CD1 ILE	250	56.707	-6.401	7.283	1.00	43.14	PROT
ATOM	343	C ILE	250	60.311	-3.590	9.294	1.00	45.32	PROT
ATOM	344	O ILE	250	60.257	-3.724	10.513	1.00	43.74	PROT
ATOM	345	N GLY	251	60.680	-2.459	8.711	1.00	36.80	PROT
ATOM	346	CA GLY	251	61.091	-1.329	9.521	1.00	39.28	PROT
ATOM	347	C GLY	251	62.370	-1.621	10.305	1.00	44.31	PROT
ATOM	348	O GLY	251	62.538	-1.145	11.428	1.00	51.39	PROT
ATOM	349	N GLN	252	63.277	-2.399	9.715	1.00	55.47	PROT
ATOM	350	CA GLN	252	64.536	-2.745	10.374	1.00	54.24	PROT
ATOM	351	CB GLN	252	64.792	-4.237	10.245	1.00	49.31	PROT
ATOM	352	C GLN	252	65.720	-1.959	9.812	1.00	54.86	PROT
ATOM	353	O GLN	252	65.492	-1.079	8.953	1.00	58.80	PROT
ATOM	354	CB VAL	264	60.887	6.759	5.510	1.00	34.33	PROT
ATOM	355	CG1 VAL	264	59.550	6.086	5.790	1.00	34.34	PROT
ATOM	356	CG2 VAL	264	60.893	8.163	6.080	1.00	20.22	PROT
ATOM	357	C VAL	264	62.053	4.557	5.439	1.00	34.08	PROT
ATOM	358	O VAL	264	62.280	4.466	4.232	1.00	46.39	PROT
ATOM	359	N VAL	264	63.361	6.605	5.966	1.00	21.27	PROT
ATOM	360	CA VAL	264	62.041	5.920	6.122	1.00	29.68	PROT
ATOM	361	N ASP	265	61.809	3.499	6.209	1.00	40.63	PROT
ATOM	362	CA ASP	265	61.796	2.141	5.670	1.00	43.58	PROT
ATOM	363	CB ASP	265	61.243	1.160	6.704	1.00	44.07	PROT
ATOM	364	CG ASP	265	61.179	-0.262	6.185	1.00	49.19	PROT
ATOM	365	OD1 ASP	265	62.223	-0.945	6.175	1.00	57.67	PROT
ATOM	366	OD2 ASP	265	60.082	-0.702	5.789	1.00	54.75	PROT
ATOM	367	C ASP	265	60.956	2.071	4.401	1.00	48.03	PROT
ATOM	368	O ASP	265	61.362	1.458	3.411	1.00	57.44	PROT
ATOM	369	N LEU	266	59.793	2.711	4.436	1.00	40.55	PROT
ATOM	370	CA LEU	266	58.879	2.741	3.295	1.00	45.78	PROT
ATOM	371	CB LEU	266	59.638	2.962	1.977	1.00	45.92	PROT
ATOM	372	CG LEU	266	59.881	4.407	1.506	1.00	48.41	PROT
ATOM	373	CD1 LEU	266	59.934	4.432	-0.007	1.00	32.83	PROT
ATOM	374	CD2 LEU	266	58.787	5.344	2.012	1.00	45.08	PROT
ATOM	375	C LEU	266	58.064	1.462	3.214	1.00	45.45	PROT
ATOM	376	O LEU	266	56.862	1.503	2.949	1.00	42.92	PROT
ATOM	377	N GLU							

ATOM	378	CA	GLU	267	57.986	-0.935	3.415	1.00	44.34	PROT
ATOM	379	CB	GLU	267	58.943	-2.123	3.505	1.00	39.42	PROT
ATOM	380	CG	GLU	267	58.291	-3.457	3.188	1.00	40.68	PROT
ATOM	381	CD	GLU	267	58.929	-4.607	3.943	1.00	63.54	PROT
ATOM	382	OE1	GLU	267	60.103	-4.470	4.361	1.00	68.92	PROT
ATOM	383	OE2	GLU	267	58.258	-5.650	4.120	1.00	66.66	PROT
ATOM	384	C	GLU	267	57.106	-0.880	4.655	1.00	41.57	PROT
ATOM	385	O	GLU	267	55.991	-1.398	4.673	1.00	48.68	PROT
ATOM	386	N	ALA	268	57.620	-0.215	5.686	1.00	39.33	PROT
ATOM	387	CA	ALA	268	56.916	-0.057	6.951	1.00	31.62	PROT
ATOM	388	CB	ALA	268	57.918	0.134	8.063	1.00	7.56	PROT
ATOM	389	C	ALA	268	55.960	1.135	6.888	1.00	25.96	PROT
ATOM	390	O	ALA	268	54.786	1.036	7.237	1.00	17.35	PROT
ATOM	391	N	PHE	269	56.464	2.274	6.446	1.00	11.34	PROT
ATOM	392	CA	PHE	269	55.615	3.453	6.335	1.00	15.72	PROT
ATOM	393	CB	PHE	269	56.274	4.474	5.405	1.00	20.08	PROT
ATOM	394	CG	PHE	269	55.552	5.788	5.334	1.00	24.67	PROT
ATOM	395	CD1	PHE	269	55.661	6.713	6.369	1.00	15.69	PROT
ATOM	396	CD2	PHE	269	54.772	6.111	4.222	1.00	20.64	PROT
ATOM	397	CE1	PHE	269	55.003	7.942	6.300	1.00	22.55	PROT
ATOM	398	CE2	PHE	269	54.108	7.342	4.143	1.00	19.77	PROT
ATOM	399	CZ	PHE	269	54.224	8.257	5.186	1.00	19.27	PROT
ATOM	400	C	PHE	269	54.277	3.010	5.754	1.00	19.45	PROT
ATOM	401	O	PHE	269	53.212	3.351	6.261	1.00	13.40	PROT
ATOM	402	N	SER	270	54.367	2.214	4.692	1.00	43.85	PROT
ATOM	403	CA	SER	270	53.217	1.686	3.967	1.00	46.67	PROT
ATOM	404	CB	SER	270	53.687	0.669	2.924	1.00	53.60	PROT
ATOM	405	OG	SER	270	52.662	0.382	1.988	1.00	68.82	PROT
ATOM	406	C	SER	270	52.181	1.039	4.865	1.00	43.32	PROT
ATOM	407	O	SER	270	51.024	1.459	4.893	1.00	43.87	PROT
ATOM	408	N	HIS	271	52.594	0.009	5.590	1.00	34.59	PROT
ATOM	409	CA	HIS	271	51.681	-0.694	6.486	1.00	37.12	PROT
ATOM	410	CB	HIS	271	52.441	-1.772	7.266	1.00	46.61	PROT
ATOM	411	CG	HIS	271	52.603	-3.056	6.512	1.00	63.99	PROT
ATOM	412	CD2	HIS	271	51.879	-4.201	6.533	1.00	62.06	PROT
ATOM	413	ND1	HIS	271	53.608	-3.256	5.590	1.00	60.86	PROT
ATOM	414	CE1	HIS	271	53.497	-4.467	5.075	1.00	60.70	PROT
ATOM	415	NE2	HIS	271	52.456	-5.061	5.630	1.00	64.10	PROT
ATOM	416	C	HIS	271	50.973	0.261	7.459	1.00	36.53	PROT
ATOM	417	O	HIS	271	49.744	0.245	7.586	1.00	37.75	PROT
ATOM	418	N	PHE	272	51.752	1.099	8.133	1.00	32.81	PROT
ATOM	419	CA	PHE	272	51.190	2.038	9.085	1.00	27.77	PROT
ATOM	420	CB	PHE	272	52.302	2.886	9.714	1.00	10.49	PROT
ATOM										



ATOM	424	CE1 PHE	272	55.634	1.764	11.163	1.00	7.86	PROT
ATOM	425	CE2 PHE	272	53.930	0.242	11.909	1.00	6.13	PROT
ATOM	426	CZ PHE	272	55.263	0.645	11.895	1.00	8.93	PROT
ATOM	427	C PHE	272	50.168	2.939	8.405	1.00	30.96	PROT
ATOM	428	O PHE	272	49.071	3.156	8.931	1.00	30.21	PROT
ATOM	429	N THR	273	50.522	3.452	7.231	1.00	31.55	PROT
ATOM	430	CA THR	273	49.633	4.343	6.487	1.00	33.39	PROT
ATOM	431	CB THR	273	50.335	4.912	5.243	1.00	36.80	PROT
ATOM	432	OG1 THR	273	50.649	3.847	4.332	1.00	27.42	PROT
ATOM	433	CG2 THR	273	51.613	5.641	5.656	1.00	32.25	PROT
ATOM	434	C THR	273	48.350	3.647	6.056	1.00	34.07	PROT
ATOM	435	O THR	273	47.362	4.294	5.697	1.00	17.11	PROT
ATOM	436	N LYS	274	48.372	2.321	6.088	1.00	34.47	PROT
ATOM	437	CA LYS	274	47.196	1.555	5.726	1.00	42.17	PROT
ATOM	438	CB LYS	274	47.544	0.069	5.615	1.00	40.02	PROT
ATOM	439	C LYS	274	46.153	1.778	6.818	1.00	41.47	PROT
ATOM	440	O LYS	274	45.115	2.402	6.584	1.00	47.37	PROT
ATOM	441	N ILE	275	46.456	1.290	8.019	1.00	34.08	PROT
ATOM	442	CA ILE	275	45.559	1.403	9.166	1.00	25.49	PROT
ATOM	443	CB ILE	275	45.991	0.435	10.262	1.00	19.72	PROT
ATOM	444	CG2 ILE	275	46.290	-0.934	9.642	1.00	23.39	PROT
ATOM	445	CG1 ILE	275	47.249	0.958	10.953	1.00	12.96	PROT
ATOM	446	CD1 ILE	275	47.970	-0.103	11.769	1.00	11.07	PROT
ATOM	447	C ILE	275	45.440	2.805	9.762	1.00	20.03	PROT
ATOM	448	O ILE	275	44.541	3.081	10.547	1.00	18.98	PROT
ATOM	449	N ILE	276	46.347	3.694	9.402	1.00	8.88	PROT
ATOM	450	CA ILE	276	46.268	5.043	9.924	1.00	6.62	PROT
ATOM	451	CB ILE	276	47.298	5.972	9.261	1.00	21.77	PROT
ATOM	452	CG2 ILE	276	46.894	6.267	7.831	1.00	27.28	PROT
ATOM	453	CG1 ILE	276	47.374	7.288	10.028	1.00	6.75	PROT
ATOM	454	CD1 ILE	276	48.349	7.255	11.153	1.00	15.44	PROT
ATOM	455	C ILE	276	44.887	5.649	9.697	1.00	12.17	PROT
ATOM	456	O ILE	276	44.349	6.331	10.565	1.00	29.36	PROT
ATOM	457	N THR	277	44.303	5.411	8.535	1.00	22.12	PROT
ATOM	458	CA THR	277	43.007	6.005	8.260	1.00	27.16	PROT
ATOM	459	CB THR	277	42.532	5.675	6.834	1.00	27.11	PROT
ATOM	460	OG1 THR	277	43.665	5.584	5.955	1.00	22.55	PROT
ATOM	461	CG2 THR	277	41.594	6.763	6.337	1.00	26.98	PROT
ATOM	462	C THR	277	41.944	5.591	9.270	1.00	25.23	PROT
ATOM	463	O THR	277	41.271	6.443	9.847	1.00	21.62	PROT
ATOM	464	N PRO	278	41.769	4.279	9.491	1.00	18.64	PROT
ATOM	465	CD PRO	278	42.472	3.167	8.832	1.00	9.52	PROT
ATOM	466	CA PRO	278	40.765	3.803	10.453	1.00	18.48	PROT
ATOM	467	CB PRO	278	40.907	2.280	10.415	1.00	14.77	PROT
ATOM	468	CG PRO	278	42.195	2.008	9.738	1.00	7.70	PROT
ATOM	469	C PRO	278	40.956	4.356	11.870	1.00	25.40	PROT



ATOM	470	O	PRO	278	39.983	4.628	12.576	1.00	22.33	PROT
ATOM	471	N	ALA	279	42.211	4.507	12.285	1.00	22.14	PROT
ATOM	472	CA	ALA	279	42.519	5.038	13.607	1.00	20.26	PROT
ATOM	473	CB	ALA	279	44.016	5.033	13.831	1.00	13.33	PROT
ATOM	474	C	ALA	279	41.984	6.456	13.699	1.00	16.49	PROT
ATOM	475	O.	ALA	279	41.222	6.797	14.598	1.00	32.38	PROT
ATOM	476	N	ILE	280	42.384	7.286	12.753	1.00	7.56	PROT
ATOM	477	CA	ILE	280	41.935	8.666	12.734	1.00	9.96	PROT
ATOM	478	CB	ILE	280	42.422	9.380	11.462	1.00	8.46	PROT
ATOM	479	CG2	ILE	280	42.172	10.871	11.581	1.00	2.00	PROT
ATOM	480	CG1	ILE	280	43.901	9.059	11.220	1.00	10.96	PROT
ATOM	481	CD1	ILE	280	44.615	10.036	10.294	1.00	8.54	PROT
ATOM	482	C	ILE	280	40.410	8.805	12.805	1.00	15.46	PROT
ATOM	483	O	ILE	280	39.887	9.741	13.421	1.00	24.39	PROT
ATOM	484	N	THR	281	39.692	7.883	12.172	1.00	24.18	PROT
ATOM	485	CA	THR	281	38.238	7.962	12.153	1.00	24.77	PROT
ATOM	486	CB	THR	281	37.650	6.952	11.145	1.00	33.90	PROT
ATOM	487	OG1	THR	281	38.607	6.711	10.108	1.00	34.62	PROT
ATOM	488	CG2	THR	281	36.379	7.506	10.513	1.00	39.80	PROT
ATOM	489	C	THR	281	37.655	7.726	13.535	1.00	23.39	PROT
ATOM	490	O	THR	281	36.733	8.422	13.960	1.00	19.51	PROT
ATOM	491	N	ARG	282	38.213	6.743	14.234	1.00	16.90	PROT
ATOM	492	CA	ARG	282	37.781	6.404	15.583	1.00	12.29	PROT
ATOM	493	CB	ARG	282	38.641	5.260	16.115	1.00	5.36	PROT
ATOM	494	CG	ARG	282	37.936	3.926	16.136	1.00	17.05	PROT
ATOM	495	CD	ARG	282	38.296	3.095	14.942	1.00	18.41	PROT
ATOM	496	NE	ARG	282	39.622	2.475	15.011	1.00	35.77	PROT
ATOM	497	CZ	ARG	282	40.454	2.501	16.055	1.00	36.80	PROT
ATOM	498	NH1	ARG	282	41.629	1.888	15.967	1.00	35.96	PROT
ATOM	499	NH2	ARG	282	40.134	3.120	17.183	1.00	25.20	PROT
ATOM	500	C	ARG	282	37.863	7.626	16.520	1.00	16.75	PROT
ATOM	501	O	ARG	282	37.078	7.758	17.456	1.00	22.98	PROT
ATOM	502	N	VAL	283	38.813	8.518	16.268	1.00	11.92	PROT
ATOM	503	CA	VAL	283	38.937	9.719	17.083	1.00	14.68	PROT
ATOM	504	CB	VAL	283	40.191	10.541	16.696	1.00	23.35	PROT
ATOM	505	CG1	VAL	283	40.467	11.593	17.752	1.00	11.98	PROT
ATOM	506	CG2	VAL	283	41.396	9.621	16.526	1.00	20.41	PROT
ATOM	507	C	VAL	283	37.705	10.580	16.833	1.00	12.72	PROT
ATOM	508	O	VAL	283	36.965	10.929	17.752	1.00	20.37	PROT
ATOM	509	N	VAL	284	37.503	10.920	15.567	1.00	18.28	PROT
ATOM	510	CA	VAL	284	36.369	11.727	15.150	1.00	16.98	PROT
ATOM	511	CB	VAL	284	36.251	11.765	13.602	1.00	27.40	PROT
ATOM	512	CG1	VAL	284	35.434	12.973	13.172			

ATOM	516	N	ASP	285	35.046	9.768	15.623	1.00	10.68	PROT
ATOM	517	CA	ASP	285	33.898	9.022	16.114	1.00	20.76	PROT
ATOM	518	CB	ASP	285	34.079	7.518	15.874	1.00	22.99	PROT
ATOM	519	CG	ASP	285	33.985	7.130	14.397	1.00	30.01	PROT
ATOM	520	OD1	ASP	285	33.185	7.735	13.648	1.00	18.56	PROT
ATOM	521	OD2	ASP	285	34.720	6.202	13.993	1.00	27.74	PROT
ATOM	522	C	ASP	285	33.734	9.274	17.604	1.00	26.87	PROT
ATOM	523	O	ASP	285	32.609	9.349	18.103	1.00	39.89	PROT
ATOM	524	N	PHE	286	34.861	9.405	18.308	1.00	25.45	PROT
ATOM	525	CA	PHE	286	34.862	9.654	19.746	1.00	15.66	PROT
ATOM	526	CB	PHE	286	36.284	9.533	20.305	1.00	7.30	PROT
ATOM	527	CG	PHE	286	36.454	10.104	21.703	1.00	17.92	PROT
ATOM	528	CD1	PHE	286	35.848	9.499	22.805	1.00	19.35	PROT
ATOM	529	CD2	PHE	286	37.229	11.245	21.920	1.00	19.24	PROT
ATOM	530	CE1	PHE	286	36.014	10.021	24.087	1.00	9.94	PROT
ATOM	531	CE2	PHE	286	37.395	11.769	23.207	1.00	11.33	PROT
ATOM	532	CZ	PHE	286	36.786	11.154	24.283	1.00	2.00	PROT
ATOM	533	C	PHE	286	34.313	11.043	20.030	1.00	17.67	PROT
ATOM	534	O	PHE	286	33.367	11.201	20.797	1.00	14.36	PROT
ATOM	535	N	ALA	287	34.905	12.056	19.410	1.00	12.57	PROT
ATOM	536	CA	ALA	287	34.443	13.426	19.622	1.00	12.49	PROT
ATOM	537	CB	ALA	287	35.250	14.386	18.759	1.00	23.54	PROT
ATOM	538	C	ALA	287	32.954	13.559	19.307	1.00	9.21	PROT
ATOM	539	O	ALA	287	32.209	14.205	20.043	1.00	11.68	PROT
ATOM	540	N	LYS	288	32.540	12.929	18.209	1.00	16.43	PROT
ATOM	541	CA	LYS	288	31.157	12.944	17.736	1.00	16.10	PROT
ATOM	542	CB	LYS	288	31.003	11.977	16.569	1.00	13.15	PROT
ATOM	543	CG	LYS	288	31.117	12.636	15.219	1.00	25.55	PROT
ATOM	544	CD	LYS	288	30.480	11.779	14.136	1.00	32.95	PROT
ATOM	545	CE	LYS	288	31.279	10.507	13.900	1.00	34.58	PROT
ATOM	546	NZ	LYS	288	30.755	9.721	12.748	1.00	36.93	PROT
ATOM	547	C	LYS	288	30.154	12.569	18.813	1.00	18.87	PROT
ATOM	548	O	LYS	288	29.078	13.171	18.917	1.00	12.83	PROT
ATOM	549	N	LYS	289	30.525	11.574	19.614	1.00	11.81	PROT
ATOM	550	CA	LYS	289	29.674	11.067	20.681	1.00	15.53	PROT
ATOM	551	CB	LYS	289	30.070	9.631	21.011	1.00	15.88	PROT
ATOM	552	CG	LYS	289	29.767	8.645	19.911	1.00	20.93	PROT
ATOM	553	CD	LYS	289	29.140	7.382	20.471	1.00	28.97	PROT
ATOM	554	CE	LYS	289	29.951	6.167	20.071	1.00	25.06	PROT
ATOM	555	NZ	LYS	289	30.043	6.060	18.590	1.00	39.19	PROT
ATOM	556	C	LYS	289	29.660	11.884	21.969	1.00	15.95	PROT
ATOM	557	O	LYS	289	29.205	11.398	23.001	1.00	28.53	PROT
ATOM	558	N	LEU	290						

ATOM	562	CD1 LEU	290	34.016	13.900	23.678	1.00	3.02	PROT
ATOM	563	CD2 LEU	290	32.449	12.257	24.686	1.00	9.39	PROT
ATOM	564	C LEU	290	29.410	15.259	22.849	1.00	7.59	PROT
ATOM	565	O LEU	290	29.942	16.148	22.196	1.00	11.01	PROT
ATOM	566	N PRO	291	28.169	15.381	23.365	1.00	14.33	PROT
ATOM	567	CD PRO	291	27.515	14.291	24.109	1.00	18.52	PROT
ATOM	568	CA PRO	291	27.290	16.556	23.240	1.00	6.61	PROT
ATOM	569	CB PRO	291	26.296	16.400	24.384	1.00	11.95	PROT
ATOM	570	CG PRO	291	26.496	15.004	24.929	1.00	20.22	PROT
ATOM	571	C PRO	291	28.029	17.885	23.332	1.00	14.74	PROT
ATOM	572	O PRO	291	27.795	18.792	22.537	1.00	26.09	PROT
ATOM	573	N MET	292	28.917	18.002	24.315	1.00	24.06	PROT
ATOM	574	CA MET	292	29.697	19.225	24.494	1.00	25.33	PROT
ATOM	575	CB MET	292	30.706	19.046	25.628	1.00	26.65	PROT
ATOM	576	CG MET	292	30.222	19.581	26.962	1.00	26.97	PROT
ATOM	577	SD MET	292	31.153	18.943	28.362	1.00	29.01	PROT
ATOM	578	CE MET	292	30.315	17.438	28.685	1.00	17.91	PROT
ATOM	579	C MET	292	30.430	19.588	23.204	1.00	23.01	PROT
ATOM	580	O MET	292	30.478	20.747	22.813	1.00	31.98	PROT
ATOM	581	N PHE	293	31.007	18.591	22.547	1.00	23.44	PROT
ATOM	582	CA PHE	293	31.724	18.819	21.297	1.00	24.83	PROT
ATOM	583	CB PHE	293	32.389	17.529	20.830	1.00	15.05	PROT
ATOM	584	CG PHE	293	33.214	17.686	19.594	1.00	13.55	PROT
ATOM	585	CD1 PHE	293	34.376	18.446	19.614	1.00	19.86	PROT
ATOM	586	CD2 PHE	293	32.867	17.024	18.425	1.00	22.99	PROT
ATOM	587	CE1 PHE	293	35.184	18.540	18.495	1.00	18.15	PROT
ATOM	588	CE2 PHE	293	33.671	17.108	17.291	1.00	20.83	PROT
ATOM	589	CZ PHE	293	34.831	17.866	17.328	1.00	22.53	PROT
ATOM	590	C PHE	293	30.759	19.291	20.222	1.00	27.26	PROT
ATOM	591	O PHE	293	30.971	20.319	19.577	1.00	28.69	PROT
ATOM	592	N CYS	294	29.689	18.528	20.040	1.00	29.92	PROT
ATOM	593	CA CYS	294	28.700	18.855	19.037	1.00	35.54	PROT
ATOM	594	CB CYS	294	27.540	17.860	19.106	1.00	19.11	PROT
ATOM	595	SG CYS	294	27.843	16.358	18.132	1.00	35.66	PROT
ATOM	596	C CYS	294	28.203	20.291	19.171	1.00	38.84	PROT
ATOM	597	O CYS	294	28.072	20.995	18.169	1.00	45.94	PROT
ATOM	598	N GLU	295	27.959	20.739	20.401	1.00	27.34	PROT
ATOM	599	CA GLU	295	27.472	22.097	20.632	1.00	21.06	PROT
ATOM	600	CB GLU	295	27.178	22.306	22.121	1.00	29.78	PROT
ATOM	601	C GLU	295	28.458	23.158	20.128	1.00	23.67	PROT
ATOM	602	O GLU	295	28.228	24.357	20.272	1.00	29.89	PROT
ATOM	603	N LEU	296	29.551	22.715	19.522	1.00	21.46	PROT
ATOM	604	CA LEU	296	30.545	23.642	19.005	1.00	26.35	PROT
ATOM	605	CB LEU	296	31.947	23.128	19.330	1.00	25.17	PROT
ATOM	606	CG LEU	296						





ATOM	654	CG1	ILE	302	36.656	20.610	10.941	1.00	29.63	PROT
ATOM	655	CD1	ILE	302	36.296	21.356	9.698	1.00	32.99	PROT
ATOM	656	C	ILE	302	39.308	21.014	13.670	1.00	28.73	PROT
ATOM	657	O	ILE	302	40.219	20.219	13.895	1.00	36.02	PROT
ATOM	658	N	ILE	303	39.396	22.304	13.968	1.00	25.04	PROT
ATOM	659	CA	ILE	303	40.590	22.817	14.603	1.00	24.27	PROT
ATOM	660	CB	ILE	303	40.414	24.270	15.054	1.00	20.89	PROT
ATOM	661	CG2	ILE	303	41.686	24.740	15.744	1.00	32.38	PROT
ATOM	662	CG1	ILE	303	40.079	25.158	13.849	1.00	18.88	PROT
ATOM	663	CD1	ILE	303	40.298	26.648	14.079	1.00	5.31	PROT
ATOM	664	C	ILE	303	40.861	21.948	15.825	1.00	26.92	PROT
ATOM	665	O	ILE	303	41.963	21.440	15.997	1.00	31.32	PROT
ATOM	666	N	LEU	304	39.843	21.763	16.659	1.00	11.00	PROT
ATOM	667	CA	LEU	304	39.983	20.953	17.854	1.00	7.21	PROT
ATOM	668	CB	LEU	304	38.663	20.886	18.613	1.00	2.00	PROT
ATOM	669	CG	LEU	304	38.633	21.511	20.012	1.00	8.04	PROT
ATOM	670	CD1	LEU	304	39.383	22.812	19.997	1.00	2.00	PROT
ATOM	671	CD2	LEU	304	37.188	21.729	20.472	1.00	4.99	PROT
ATOM	672	C	LEU	304	40.441	19.554	17.507	1.00	4.64	PROT
ATOM	673	O	LEU	304	41.368	19.032	18.119	1.00	14.88	PROT
ATOM	674	N	LEU	305	39.807	18.953	16.510	1.00	4.55	PROT
ATOM	675	CA	LEU	305	40.140	17.590	16.093	1.00	7.03	PROT
ATOM	676	CB	LEU	305	39.099	17.098	15.104	1.00	3.70	PROT
ATOM	677	CG	LEU	305	38.164	16.054	15.691	1.00	10.31	PROT
ATOM	678	CD1	LEU	305	36.744	16.340	15.245	1.00	2.00	PROT
ATOM	679	CD2	LEU	305	38.629	14.665	15.260	1.00	9.42	PROT
ATOM	680	C	LEU	305	41.527	17.418	15.483	1.00	10.17	PROT
ATOM	681	O	LEU	305	42.174	16.374	15.651	1.00	7.58	PROT
ATOM	682	N	LYS	306	41.975	18.442	14.765	1.00	9.98	PROT
ATOM	683	CA	LYS	306	43.283	18.408	14.127	1.00	9.14	PROT
ATOM	684	CB	LYS	306	43.409	19.558	13.131	1.00	18.85	PROT
ATOM	685	CG	LYS	306	42.815	19.270	11.763	1.00	25.44	PROT
ATOM	686	CD	LYS	306	42.198	20.529	11.178	1.00	29.07	PROT
ATOM	687	CE	LYS	306	42.698	20.808	9.774	1.00	37.81	PROT
ATOM	688	NZ	LYS	306	43.867	19.964	9.403	1.00	30.48	PROT
ATOM	689	C	LYS	306	44.376	18.522	15.175	1.00	7.31	PROT
ATOM	690	O	LYS	306	45.439	17.919	15.048	1.00	16.95	PROT
ATOM	691	N	GLY	307	44.097	19.295	16.218	1.00	12.67	PROT
ATOM	692	CA	GLY	307	45.062	19.484	17.279	1.00	7.25	PROT
ATOM	693	C	GLY	307	45.297	18.269	18.150	1.00	15.08	PROT
ATOM	694	O	GLY	307	46.441	17.972	18.488	1.00	20.11	PROT
ATOM	695	N	CYS	308	44.225	17.552	18.481	1.00	8.29	PROT
ATOM	696	CA								



ATOM	700	O	CYS	308	44.502	13.997	19.453	1.00	10.98	PROT
ATOM	701	N	CYS	309	44.202	14.916	17.420	1.00	10.83	PROT
ATOM	702	CA	CYS	309	44.236	13.625	16.752	1.00	3.22	PROT
ATOM	703	CB	CYS	309	44.240	13.831	15.240	1.00	15.79	PROT
ATOM	704	SG	CYS	309	43.683	12.402	14.319	1.00	25.54	PROT
ATOM	705	C-	CYS	309	45.439	12.767	17.193	1.00	2.00	PROT
ATOM	706	O	CYS	309	45.251	11.722	17.807	1.00	12.28	PROT
ATOM	707	N	MET	310	46.663	13.205	16.900	1.00	2.00	PROT
ATOM	708	CA	MET	310	47.858	12.446	17.286	1.00	2.00	PROT
ATOM	709	CB	MET	310	49.122	13.171	16.860	1.00	2.00	PROT
ATOM	710	CG	MET	310	49.975	12.422	15.880	1.00	5.92	PROT
ATOM	711	SD	MET	310	50.481	10.805	16.368	1.00	22.47	PROT
ATOM	712	CE	MET	310	52.140	11.112	16.808	1.00	20.84	PROT
ATOM	713	C	MET	310	47.941	12.239	18.793	1.00	11.95	PROT
ATOM	714	O	MET	310	48.455	11.220	19.270	1.00	15.53	PROT
ATOM	715	N	GLU	311	47.463	13.225	19.542	1.00	6.79	PROT
ATOM	716	CA	GLU	311	47.493	13.139	20.979	1.00	2.00	PROT
ATOM	717	CB	GLU	311	46.932	14.427	21.581	1.00	6.42	PROT
ATOM	718	CG	GLU	311	47.880	15.619	21.436	1.00	8.40	PROT
ATOM	719	CD	GLU	311	47.236	16.940	21.820	1.00	14.10	PROT
ATOM	720	OE1	GLU	311	46.157	16.895	22.434	1.00	16.54	PROT
ATOM	721	OE2	GLU	311	47.795	18.020	21.515	1.00	4.09	PROT
ATOM	722	C	GLU	311	46.683	11.923	21.406	1.00	7.80	PROT
ATOM	723	O	GLU	311	47.195	11.026	22.067	1.00	14.07	PROT
ATOM	724	N	ILE	312	45.425	11.873	21.001	1.00	2.00	PROT
ATOM	725	CA	ILE	312	44.574	10.752	21.371	1.00	3.60	PROT
ATOM	726	CB	ILE	312	43.114	11.013	20.947	1.00	2.00	PROT
ATOM	727	CG2	ILE	312	42.277	9.769	21.145	1.00	2.00	PROT
ATOM	728	CG1	ILE	312	42.579	12.221	21.727	1.00	2.00	PROT
ATOM	729	CD1	ILE	312	41.118	12.555	21.495	1.00	2.00	PROT
ATOM	730	C	ILE	312	45.049	9.437	20.760	1.00	8.32	PROT
ATOM	731	O	ILE	312	44.918	8.373	21.370	1.00	5.58	PROT
ATOM	732	N	MET	313	45.615	9.501	19.563	1.00	3.98	PROT
ATOM	733	CA	MET	313	46.054	8.282	18.905	1.00	8.91	PROT
ATOM	734	CB	MET	313	46.455	8.572	17.462	1.00	25.71	PROT
ATOM	735	CG	MET	313	45.430	8.111	16.431	1.00	22.86	PROT
ATOM	736	SD	MET	313	45.955	8.430	14.736	1.00	20.60	PROT
ATOM	737	CE	MET	313	45.412	10.055	14.534	1.00	14.95	PROT
ATOM	738	C	MET	313	47.211	7.634	19.635	1.00	12.95	PROT
ATOM	739	O	MET	313	47.213	6.426	19.857	1.00	22.09	PROT
ATOM	740	N	SER	314	48.190	8.442	20.021	1.00	10.79	PROT
ATOM	741	CA	SER	314	49.354	7.935	20.719	1.00	2.00	PROT
ATOM	742	CB	SER	314	50.399	9.042				

ATOM	746	N	LEU	315	48.050	8.062	22.782	1.00	2.00	PROT
ATOM	747	CA	LEU	315	47.628	7.605	24.104	1.00	2.00	PROT
ATOM	748	CB	LEU	315	46.521	8.502	24.671	1.00	2.95	PROT
ATOM	749	CG	LEU	315	45.831	8.096	25.992	1.00	2.00	PROT
ATOM	750	CD1	LEU	315	46.876	7.845	27.072	1.00	2.54	PROT
ATOM	751	CD2	LEU	315	44.865	9.182	26.444	1.00	2.00	PROT
ATOM	752	C	LEU	315	47.107	6.182	23.945	1.00	3.25	PROT
ATOM	753	O	LEU	315	47.568	5.253	24.603	1.00	2.00	PROT
ATOM	754	N	ARG	316	46.157	6.010	23.039	1.00	7.28	PROT
ATOM	755	CA	ARG	316	45.588	4.691	22.808	1.00	13.31	PROT
ATOM	756	CB	ARG	316	44.551	4.758	21.693	1.00	11.11	PROT
ATOM	757	CG	ARG	316	43.545	5.872	21.887	1.00	10.55	PROT
ATOM	758	CD	ARG	316	42.354	5.639	21.012	1.00	10.09	PROT
ATOM	759	NE	ARG	316	41.131	6.149	21.605	1.00	12.29	PROT
ATOM	760	CZ	ARG	316	39.955	6.127	20.994	1.00	6.99	PROT
ATOM	761	NH1	ARG	316	38.880	6.608	21.595	1.00	19.32	PROT
ATOM	762	NH2	ARG	316	39.853	5.619	19.778	1.00	17.16	PROT
ATOM	763	C	ARG	316	46.666	3.686	22.458	1.00	10.10	PROT
ATOM	764	O	ARG	316	46.549	2.508	22.753	1.00	14.94	PROT
ATOM	765	N	ALA	317	47.723	4.148	21.819	1.00	6.51	PROT
ATOM	766	CA	ALA	317	48.801	3.243	21.474	1.00	11.04	PROT
ATOM	767	CB	ALA	317	49.749	3.902	20.487	1.00	16.13	PROT
ATOM	768	C	ALA	317	49.539	2.910	22.753	1.00	12.70	PROT
ATOM	769	O	ALA	317	49.822	1.755	23.033	1.00	23.09	PROT
ATOM	770	N	ALA	318	49.832	3.943	23.534	1.00	14.79	PROT
ATOM	771	CA	ALA	318	50.567	3.779	24.776	1.00	8.38	PROT
ATOM	772	CB	ALA	318	50.727	5.122	25.448	1.00	11.75	PROT
ATOM	773	C	ALA	318	49.941	2.786	25.741	1.00	10.30	PROT
ATOM	774	O	ALA	318	50.585	1.824	26.165	1.00	8.48	PROT
ATOM	775	N	VAL	319	48.680	3.011	26.083	1.00	7.87	PROT
ATOM	776	CA	VAL	319	48.002	2.131	27.027	1.00	9.64	PROT
ATOM	777	CB	VAL	319	46.579	2.622	27.334	1.00	2.57	PROT
ATOM	778	CG1	VAL	319	46.644	3.929	28.127	1.00	5.09	PROT
ATOM	779	CG2	VAL	319	45.807	2.823	26.043	1.00	5.15	PROT
ATOM	780	C	VAL	319	47.930	0.695	26.541	1.00	11.68	PROT
ATOM	781	O	VAL	319	47.440	-0.171	27.254	1.00	16.32	PROT
ATOM	782	N	ARG	320	48.415	0.444	25.329	1.00	16.40	PROT
ATOM	783	CA	ARG	320	48.405	-0.902	24.767	1.00	13.20	PROT
ATOM	784	CB	ARG	320	47.736	-0.918	23.393	1.00	2.00	PROT
ATOM	785	CG	ARG	320	46.310	-0.405	23.420	1.00	14.07	PROT
ATOM	786	CD	ARG	320	45.283	-1.460	23.035	1.00	19.69	PROT
ATOM	787	NE	ARG	320	44.168	-0.868	22.292	1.00	36.52	PROT
ATOM	788	CZ	ARG	320	42.912	-1.313	22.322	1.00	47.4	

ATOM	792	O	ARG	320	50.167	-2.218	23.809	1.00	24.78	PROT
ATOM	793	N	TYR	321	50.684	-0.860	25.537	1.00	13.68	PROT
ATOM	794	CA	TYR	321	52.085	-1.258	25.572	1.00	18.80	PROT
ATOM	795	CB	TYR	321	52.925	-0.208	26.295	1.00	9.64	PROT
ATOM	796	CG	TYR	321	54.313	-0.685	26.622	1.00	11.20	PROT
ATOM	797	CD1	TYR	321	55.211	-1.005	25.612	1.00	2.00	PROT
ATOM	798	CE1	TYR	321	56.483	-1.461	25.906	1.00	9.63	PROT
ATOM	799	CD2	TYR	321	54.727	-0.834	27.943	1.00	18.93	PROT
ATOM	800	CE2	TYR	321	56.003	-1.293	28.250	1.00	19.49	PROT
ATOM	801	CZ	TYR	321	56.874	-1.604	27.225	1.00	14.75	PROT
ATOM	802	OH	TYR	321	58.137	-2.053	27.518	1.00	22.96	PROT
ATOM	803	C	TYR	321	52.209	-2.607	26.287	1.00	19.74	PROT
ATOM	804	O	TYR	321	51.483	-2.889	27.242	1.00	31.56	PROT
ATOM	805	N	ASP	322	53.136	-3.435	25.823	1.00	26.35	PROT
ATOM	806	CA	ASP	322	53.346	-4.759	26.392	1.00	22.38	PROT
ATOM	807	CB	ASP	322	52.982	-5.814	25.353	1.00	33.63	PROT
ATOM	808	CG	ASP	322	52.601	-7.128	25.970	1.00	40.70	PROT
ATOM	809	OD1	ASP	322	51.539	-7.658	25.591	1.00	48.18	PROT
ATOM	810	OD2	ASP	322	53.358	-7.628	26.826	1.00	38.91	PROT
ATOM	811	C	ASP	322	54.800	-4.928	26.776	1.00	23.51	PROT
ATOM	812	O	ASP	322	55.683	-4.844	25.924	1.00	37.80	PROT
ATOM	813	N	PRO	323	55.076	-5.160	28.066	1.00	24.06	PROT
ATOM	814	CD	PRO	323	54.130	-5.258	29.187	1.00	19.35	PROT
ATOM	815	CA	PRO	323	56.462	-5.339	28.507	1.00	23.60	PROT
ATOM	816	CB	PRO	323	56.390	-5.121	30.007	1.00	3.90	PROT
ATOM	817	CG	PRO	323	55.031	-5.570	30.360	1.00	14.06	PROT
ATOM	818	C	PRO	323	56.949	-6.736	28.151	1.00	21.79	PROT
ATOM	819	O	PRO	323	58.149	-7.003	28.119	1.00	27.28	PROT
ATOM	820	N	GLU	324	56.009	-7.633	27.889	1.00	37.63	PROT
ATOM	821	CA	GLU	324	56.366	-8.993	27.524	1.00	42.63	PROT
ATOM	822	CB	GLU	324	55.133	-9.885	27.551	1.00	37.58	PROT
ATOM	823	C	GLU	324	56.971	-8.956	26.124	1.00	43.28	PROT
ATOM	824	O	GLU	324	58.154	-9.239	25.938	1.00	43.14	PROT
ATOM	825	N	SER	325	56.153	-8.586	25.142	1.00	31.72	PROT
ATOM	826	CA	SER	325	56.607	-8.508	23.765	1.00	30.34	PROT
ATOM	827	CB	SER	325	55.413	-8.522	22.814	1.00	17.63	PROT
ATOM	828	OG	SER	325	54.356	-7.729	23.315	1.00	31.90	PROT
ATOM	829	C	SER	325	57.441	-7.257	23.519	1.00	31.94	PROT
ATOM	830	O	SER	325	58.146	-7.169	22.513	1.00	45.47	PROT
ATOM	831	N	GLU	326	57.359	-6.289	24.429	1.00	31.10	PROT
ATOM	832	CA	GLU	326	58.119	-5.050	24.281	1.00	31.43	PROT
ATOM	833	CB	GLU	326	59.598	-5.382	24.091	1.00	30.39	PROT
ATOM	834	CG	GLU	326	60.552	-4.342				

ATOM	838	C	GLU	326	57.605	-4.283	23.063	1.00	28.37	PROT
ATOM	839	O	GLU	326	58.382	-3.677	22.321	1.00	26.51	PROT
ATOM	840	N	THR	327	56.290	-4.301	22.873	1.00	23.71	PROT
ATOM	841	CA	THR	327	55.674	-3.648	21.720	1.00	22.11	PROT
ATOM	842	CB	THR	327	55.298	-4.705	20.652	1.00	28.08	PROT
ATOM	843	OG1	THR	327	54.226	-5.524	21.145	1.00	16.87	PROT
ATOM	844	CG2	THR	327	56.494	-5.597	20.340	1.00	24.03	PROT
ATOM	845	C	THR	327	54.420	-2.824	22.046	1.00	22.42	PROT
ATOM	846	O	THR	327	53.928	-2.830	23.172	1.00	17.50	PROT
ATOM	847	N	LEU	328	53.914	-2.122	21.038	1.00	17.28	PROT
ATOM	848	CA	LEU	328	52.728	-1.285	21.171	1.00	14.83	PROT
ATOM	849	CB	LEU	328	53.065	0.157	20.806	1.00	15.27	PROT
ATOM	850	CG	LEU	328	53.693	1.036	21.879	1.00	10.50	PROT
ATOM	851	CD1	LEU	328	54.137	2.336	21.254	1.00	16.75	PROT
ATOM	852	CD2	LEU	328	52.682	1.285	22.979	1.00	20.19	PROT
ATOM	853	C	LEU	328	51.687	-1.804	20.198	1.00	18.16	PROT
ATOM	854	O	LEU	328	52.035	-2.508	19.254	1.00	23.88	PROT
ATOM	855	N	THR	329	50.421	-1.450	20.402	1.00	9.40	PROT
ATOM	856	CA	THR	329	49.389	-1.920	19.495	1.00	8.26	PROT
ATOM	857	CB	THR	329	48.460	-2.888	20.199	1.00	8.67	PROT
ATOM	858	OG1	THR	329	49.213	-4.052	20.577	1.00	13.23	PROT
ATOM	859	CG2	THR	329	47.308	-3.289	19.270	1.00	2.00	PROT
ATOM	860	C	THR	329	48.569	-0.841	18.800	1.00	16.65	PROT
ATOM	861	O	THR	329	47.726	-0.158	19.406	1.00	17.20	PROT
ATOM	862	N	LEU	330	48.808	-0.725	17.495	1.00	21.56	PROT
ATOM	863	CA	LEU	330	48.138	0.258	16.655	1.00	20.95	PROT
ATOM	864	CB	LEU	330	49.106	0.676	15.539	1.00	17.36	PROT
ATOM	865	CG	LEU	330	50.570	0.797	16.028	1.00	12.86	PROT
ATOM	866	CD1	LEU	330	51.531	0.521	14.898	1.00	10.10	PROT
ATOM	867	CD2	LEU	330	50.830	2.180	16.600	1.00	2.00	PROT
ATOM	868	C	LEU	330	46.803	-0.258	16.097	1.00	21.35	PROT
ATOM	869	O	LEU	330	46.655	-1.444	15.791	1.00	21.93	PROT
ATOM	870	N	ASN	331	45.834	0.648	15.987	1.00	27.76	PROT
ATOM	871	CA	ASN	331	44.487	0.338	15.498	1.00	28.09	PROT
ATOM	872	CB	ASN	331	44.460	0.275	13.971	1.00	24.95	PROT
ATOM	873	CG	ASN	331	43.074	0.540	13.397	1.00	33.45	PROT
ATOM	874	OD1	ASN	331	42.512	-0.305	12.701	1.00	38.21	PROT
ATOM	875	ND2	ASN	331	42.522	1.715	13.680	1.00	24.73	PROT
ATOM	876	C	ASN	331	43.946	-0.967	16.075	1.00	32.03	PROT
ATOM	877	O	ASN	331	43.166	-1.668	15.431	1.00	35.49	PROT
ATOM	878	N	GLY	332	44.357	-1.282	17.299	1.00	40.24	PROT
ATOM	879	CA	GLY	332	43.894	-2.495	17.941	1.00	38.04	PROT
ATOM	880	C	GLY	332	44.009	-3.665</				



ATOM	884	CB	GLU	333	44.752	-4.978	14.454	1.00	46.39	PROT
ATOM	885	CG	GLU	333	44.745	-3.580	13.862	1.00	58.03	PROT
ATOM	886	CD	GLU	333	43.883	-3.485	12.610	1.00	67.00	PROT
ATOM	887	OE1	GLU	333	44.446	-3.282	11.511	1.00	67.51	PROT
ATOM	888	OE2	GLU	333	42.644	-3.615	12.727	1.00	71.01	PROT
ATOM	889	C-	GLU	333	47.027	-5.266	15.446	1.00	33.13	PROT
ATOM	890	O	GLU	333	47.563	-6.366	15.486	1.00	27.97	PROT
ATOM	891	N	MET	334	47.692	-4.152	15.143	1.00	27.00	PROT
ATOM	892	CA	MET	334	49.111	-4.188	14.798	1.00	29.83	PROT
ATOM	893	CB	MET	334	49.416	-3.159	13.699	1.00	26.04	PROT
ATOM	894	CG	MET	334	50.561	-3.588	12.765	1.00	28.06	PROT
ATOM	895	SD	MET	334	51.263	-2.273	11.736	1.00	28.46	PROT
ATOM	896	CE	MET	334	50.021	-2.123	10.497	1.00	22.48	PROT
ATOM	897	C	MET	334	50.087	-3.995	15.959	1.00	33.52	PROT
ATOM	898	O	MET	334	50.071	-2.962	16.631	1.00	35.81	PROT
ATOM	899	N	ALA	335	50.942	-4.996	16.171	1.00	27.46	PROT
ATOM	900	CA	ALA	335	51.948	-4.976	17.234	1.00	29.69	PROT
ATOM	901	CB	ALA	335	51.966	-6.314	17.965	1.00	12.67	PROT
ATOM	902	C	ALA	335	53.336	-4.682	16.662	1.00	31.74	PROT
ATOM	903	O	ALA	335	53.943	-5.530	16.009	1.00	43.66	PROT
ATOM	904	N	VAL	336	53.848	-3.489	16.923	1.00	23.98	PROT
ATOM	905	CA	VAL	336	55.151	-3.118	16.405	1.00	21.32	PROT
ATOM	906	CB	VAL	336	55.028	-1.873	15.504	1.00	17.37	PROT
ATOM	907	CG1	VAL	336	53.945	-2.104	14.462	1.00	14.88	PROT
ATOM	908	CG2	VAL	336	54.686	-0.648	16.339	1.00	15.53	PROT
ATOM	909	C	VAL	336	56.150	-2.852	17.526	1.00	22.72	PROT
ATOM	910	O	VAL	336	55.763	-2.540	18.651	1.00	25.15	PROT
ATOM	911	N	THR	337	57.435	-3.001	17.220	1.00	19.21	PROT
ATOM	912	CA	THR	337	58.476	-2.765	18.205	1.00	20.31	PROT
ATOM	913	CB	THR	337	59.752	-3.578	17.884	1.00	14.76	PROT
ATOM	914	OG1	THR	337	59.957	-3.616	16.467	1.00	16.43	PROT
ATOM	915	CG2	THR	337	59.615	-4.995	18.393	1.00	7.08	PROT
ATOM	916	C	THR	337	58.785	-1.272	18.157	1.00	24.20	PROT
ATOM	917	O	THR	337	58.322	-0.591	17.245	1.00	28.05	PROT
ATOM	918	N	ARG	338	59.548	-0.766	19.134	1.00	27.55	PROT
ATOM	919	CA	ARG	338	59.917	0.655	19.197	1.00	16.80	PROT
ATOM	920	CB	ARG	338	60.757	0.942	20.446	1.00	17.04	PROT
ATOM	921	CG	ARG	338	61.687	2.149	20.303	1.00	9.79	PROT
ATOM	922	CD	ARG	338	62.666	2.276	21.458	1.00	2.00	PROT
ATOM	923	NE	ARG	338	61.994	2.128	22.739	1.00	20.70	PROT
ATOM	924	CZ	ARG	338	61.897	3.083	23.657	1.00	12.04	PROT
ATOM	925	NH1	ARG	338	61.261	2.840	24.784	1.00	27.11	PROT
ATOM	926	NH2	ARG	338	62.436	4.272	23.459			



ATOM	930	CA	GLY	339	62.609	0.696	16.540	1.00	32.42	PROT
ATOM	931	C	GLY	339	61.816	0.534	15.254	1.00	30.08	PROT
ATOM	932	O	GLY	339	61.932	1.342	14.328	1.00	25.82	PROT
ATOM	933	N	GLN	340	61.008	-0.520	15.192	1.00	16.60	PROT
ATOM	934	CA	GLN	340	60.191	-0.768	14.012	1.00	14.08	PROT
ATOM	935	CB	GLN	340	59.199	-1.884	14.301	1.00	5.73	PROT
ATOM	936	CG	GLN	340	58.849	-2.697	13.100	1.00	16.15	PROT
ATOM	937	CD	GLN	340	58.577	-4.141	13.442	1.00	22.46	PROT
ATOM	938	OE1	GLN	340	57.767	-4.450	14.316	1.00	30.45	PROT
ATOM	939	NE2	GLN	340	59.254	-5.040	12.749	1.00	34.19	PROT
ATOM	940	C	GLN	340	59.452	0.521	13.632	1.00	22.07	PROT
ATOM	941	O	GLN	340	59.707	1.103	12.576	1.00	21.13	PROT
ATOM	942	N	LEU	341	58.561	0.976	14.518	1.00	27.88	PROT
ATOM	943	CA	LEU	341	57.778	2.197	14.306	1.00	21.82	PROT
ATOM	944	CB	LEU	341	56.813	2.418	15.483	1.00	10.20	PROT
ATOM	945	CG	LEU	341	55.930	3.682	15.534	1.00	16.27	PROT
ATOM	946	CD1	LEU	341	54.777	3.618	14.518	1.00	13.27	PROT
ATOM	947	CD2	LEU	341	55.370	3.822	16.935	1.00	10.68	PROT
ATOM	948	C	LEU	341	58.683	3.413	14.138	1.00	13.98	PROT
ATOM	949	O	LEU	341	58.315	4.386	13.486	1.00	7.94	PROT
ATOM	950	N	LYS	342	59.867	3.361	14.734	1.00	11.48	PROT
ATOM	951	CA	LYS	342	60.804	4.465	14.613	1.00	17.77	PROT
ATOM	952	CB	LYS	342	62.063	4.213	15.459	1.00	13.58	PROT
ATOM	953	CG	LYS	342	63.219	5.173	15.140	1.00	13.27	PROT
ATOM	954	CD	LYS	342	64.173	5.358	16.319	1.00	5.44	PROT
ATOM	955	CE	LYS	342	64.500	6.829	16.546	1.00	5.47	PROT
ATOM	956	NZ	LYS	342	65.721	7.019	17.388	1.00	4.98	PROT
ATOM	957	C	LYS	342	61.184	4.579	13.141	1.00	19.97	PROT
ATOM	958	O	LYS	342	60.939	5.595	12.501	1.00	20.34	PROT
ATOM	959	N	ASN	343	61.764	3.510	12.605	1.00	26.88	PROT
ATOM	960	CA	ASN	343	62.196	3.470	11.219	1.00	22.34	PROT
ATOM	961	CB	ASN	343	62.829	2.123	10.929	1.00	4.80	PROT
ATOM	962	CG	ASN	343	64.060	1.894	11.758	1.00	18.77	PROT
ATOM	963	OD1	ASN	343	64.755	2.848	12.117	1.00	14.12	PROT
ATOM	964	ND2	ASN	343	64.340	0.634	12.083	1.00	12.72	PROT
ATOM	965	C	ASN	343	61.091	3.736	10.224	1.00	20.40	PROT
ATOM	966	O	ASN	343	61.309	4.417	9.232	1.00	20.76	PROT
ATOM	967	N	GLY	344	59.908	3.200	10.494	1.00	12.62	PROT
ATOM	968	CA	GLY	344	58.775	3.382	9.603	1.00	6.27	PROT
ATOM	969	C	GLY	344	58.229	4.796	9.451	1.00	14.56	PROT
ATOM	970	O	GLY	344	57.177	4.972	8.826	1.00	13.30	PROT
ATOM	971	N	GLY	345	58.902	5.795	10.030	1.00	16.51	PROT
ATOM	972	CA	GLY	345	58.439	7				

ATOM	976	CA	LEU	346	57.874	8.449	13.415	1.00	14.94	PROT
ATOM	977	CB	LEU	346	57.070	7.700	14.474	1.00	3.92	PROT
ATOM	978	CG	LEU	346	55.566	7.538	14.193	1.00	5.92	PROT
ATOM	979	CD1	LEU	346	54.938	6.796	15.355	1.00	2.00	PROT
ATOM	980	CD2	LEU	346	54.884	8.885	13.973	1.00	2.00	PROT
ATOM	981	C	LEU	346	59.126	9.042	14.041	1.00	14.60	PROT
ATOM	982	O	LEU	346	59.102	10.153	14.554	1.00	17.36	PROT
ATOM	983	N	GLY	347	60.226	8.312	14.001	1.00	12.09	PROT
ATOM	984	CA	GLY	347	61.455	8.828	14.581	1.00	15.62	PROT
ATOM	985	C	GLY	347	61.439	8.963	16.090	1.00	6.31	PROT
ATOM	986	O	GLY	347	60.865	8.141	16.790	1.00	13.15	PROT
ATOM	987	N	VAL	348	62.076	10.011	16.592	1.00	13.74	PROT
ATOM	988	CA	VAL	348	62.141	10.259	18.030	1.00	10.13	PROT
ATOM	989	CB	VAL	348	62.757	11.646	18.342	1.00	9.26	PROT
ATOM	990	CG1	VAL	348	61.867	12.752	17.794	1.00	2.00	PROT
ATOM	991	CG2	VAL	348	62.942	11.802	19.836	1.00	2.00	PROT
ATOM	992	C	VAL	348	60.763	10.216	18.650	1.00	6.61	PROT
ATOM	993	O	VAL	348	60.619	10.066	19.862	1.00	3.12	PROT
ATOM	994	N	VAL	349	59.746	10.358	17.816	1.00	5.51	PROT
ATOM	995	CA	VAL	349	58.386	10.342	18.306	1.00	2.00	PROT
ATOM	996	CB	VAL	349	57.421	10.886	17.260	1.00	4.46	PROT
ATOM	997	CG1	VAL	349	56.001	10.578	17.656	1.00	2.00	PROT
ATOM	998	CG2	VAL	349	57.623	12.387	17.122	1.00	2.00	PROT
ATOM	999	C	VAL	349	57.995	8.933	18.687	1.00	9.15	PROT
ATOM	1000	O	VAL	349	57.284	8.726	19.664	1.00	15.02	PROT
ATOM	1001	N	SER	350	58.446	7.943	17.933	1.00	7.42	PROT
ATOM	1002	CA	SER	350	58.087	6.590	18.315	1.00	12.87	PROT
ATOM	1003	CB	SER	350	58.695	5.561	17.382	1.00	9.48	PROT
ATOM	1004	OG	SER	350	58.529	4.269	17.931	1.00	10.82	PROT
ATOM	1005	C	SER	350	58.628	6.364	19.717	1.00	15.55	PROT
ATOM	1006	O	SER	350	57.963	5.761	20.558	1.00	25.88	PROT
ATOM	1007	N	ASP	351	59.838	6.863	19.950	1.00	16.38	PROT
ATOM	1008	CA	ASP	351	60.522	6.743	21.230	1.00	9.58	PROT
ATOM	1009	CB	ASP	351	61.861	7.469	21.176	1.00	7.32	PROT
ATOM	1010	CG	ASP	351	62.989	6.576	20.742	1.00	24.16	PROT
ATOM	1011	OD1	ASP	351	64.011	7.110	20.275	1.00	30.24	PROT
ATOM	1012	OD2	ASP	351	62.866	5.343	20.869	1.00	33.85	PROT
ATOM	1013	C	ASP	351	59.695	7.360	22.334	1.00	17.01	PROT
ATOM	1014	O	ASP	351	59.605	6.822	23.435	1.00	26.28	PROT
ATOM	1015	N	ALA	352	59.100	8.508	22.032	1.00	13.51	PROT
ATOM	1016	CA	ALA	352	58.294	9.224	23.004	1.00	5.19	PROT
ATOM	1017	CB	ALA	352	57.914	10.593	22.452	1.00	2.00	PROT
ATOM	1018	C	ALA	352	57.055	8.				

ATOM	1022	CB	ILE	353	54.468	6.626	21.381	1.00	5.87	PROT
ATOM	1023	CG2	ILE	353	53.113	6.049	21.732	1.00	2.00	PROT
ATOM	1024	CG1	ILE	353	54.349	7.831	20.428	1.00	3.91	PROT
ATOM	1025	CD1	ILE	353	53.330	7.664	19.294	1.00	2.00	PROT
ATOM	1026	C	ILE	353	55.554	5.795	23.484	1.00	12.46	PROT
ATOM	1027	O	ILE	353	54.848	5.426	24.428	1.00	11.74	PROT
ATOM	1028	N	PHE	354	56.644	5.131	23.122	1.00	19.57	PROT
ATOM	1029	CA	PHE	354	57.034	3.944	23.862	1.00	14.42	PROT
ATOM	1030	CB	PHE	354	58.256	3.270	23.209	1.00	3.70	PROT
ATOM	1031	CG	PHE	354	57.890	2.141	22.284	1.00	9.42	PROT
ATOM	1032	CD1	PHE	354	57.427	2.401	20.995	1.00	12.33	PROT
ATOM	1033	CD2	PHE	354	57.912	0.822	22.727	1.00	15.63	PROT
ATOM	1034	CE1	PHE	354	56.982	1.366	20.165	1.00	6.67	PROT
ATOM	1035	CE2	PHE	354	57.468	-0.224	21.900	1.00	16.53	PROT
ATOM	1036	CZ	PHE	354	57.002	0.053	20.620	1.00	11.61	PROT
ATOM	1037	C	PHE	354	57.322	4.346	25.307	1.00	18.55	PROT
ATOM	1038	O	PHE	354	56.796	3.740	26.233	1.00	16.67	PROT
ATOM	1039	N	ASP	355	58.125	5.392	25.491	1.00	12.83	PROT
ATOM	1040	CA	ASP	355	58.486	5.881	26.818	1.00	5.31	PROT
ATOM	1041	CB	ASP	355	59.351	7.132	26.697	1.00	9.38	PROT
ATOM	1042	CG	ASP	355	60.805	6.814	26.428	1.00	5.96	PROT
ATOM	1043	OD1	ASP	355	61.112	5.683	26.016	1.00	8.53	PROT
ATOM	1044	OD2	ASP	355	61.650	7.706	26.628	1.00	15.51	PROT
ATOM	1045	C	ASP	355	57.252	6.199	27.659	1.00	10.27	PROT
ATOM	1046	O	ASP	355	57.231	5.972	28.871	1.00	21.86	PROT
ATOM	1047	N	LEU	356	56.224	6.726	27.014	1.00	4.18	PROT
ATOM	1048	CA	LEU	356	54.988	7.061	27.697	1.00	2.07	PROT
ATOM	1049	CB	LEU	356	54.086	7.865	26.771	1.00	2.24	PROT
ATOM	1050	CG	LEU	356	52.694	8.229	27.266	1.00	3.11	PROT
ATOM	1051	CD1	LEU	356	52.771	9.317	28.323	1.00	2.00	PROT
ATOM	1052	CD2	LEU	356	51.877	8.709	26.086	1.00	2.00	PROT
ATOM	1053	C	LEU	356	54.281	5.786	28.091	1.00	9.17	PROT
ATOM	1054	O	LEU	356	53.831	5.644	29.221	1.00	14.77	PROT
ATOM	1055	N	GLY	357	54.183	4.856	27.147	1.00	13.10	PROT
ATOM	1056	CA	GLY	357	53.515	3.597	27.413	1.00	6.91	PROT
ATOM	1057	C	GLY	357	54.113	2.879	28.598	1.00	8.33	PROT
ATOM	1058	O	GLY	357	53.400	2.426	29.492	1.00	9.09	PROT
ATOM	1059	N	MET	358	55.435	2.768	28.607	1.00	12.61	PROT
ATOM	1060	CA	MET	358	56.112	2.091	29.692	1.00	10.53	PROT
ATOM	1061	CB	MET	358	57.626	2.153	29.498	1.00	5.45	PROT
ATOM	1062	CG	MET	358	58.138	1.507	28.210	1.00	15.15	PROT
ATOM	1063	SD	MET	358	59.971	1.352	28.113	1.00	17.63	PROT
ATOM	1064	CE	MET	358						

ATOM	1068	CA	SER	359	55.551	4.924	32.158	1.00	19.72	PROT
ATOM	1069	CB	SER	359	55.831	6.398	31.861	1.00	19.98	PROT
ATOM	1070	OG	SER	359	54.753	7.220	32.262	1.00	33.66	PROT
ATOM	1071	C	SER	359	54.115	4.757	32.656	1.00	22.67	PROT
ATOM	1072	O	SER	359	53.849	4.837	33.860	1.00	22.94	PROT
ATOM	1073	N	LEU	360	53.197	4.514	31.727	1.00	20.55	PROT
ATOM	1074	CA	LEU	360	51.785	4.360	32.054	1.00	17.01	PROT
ATOM	1075	CB	LEU	360	50.934	4.578	30.802	1.00	2.60	PROT
ATOM	1076	CG	LEU	360	50.674	5.988	30.291	1.00	6.99	PROT
ATOM	1077	CD1	LEU	360	49.589	5.935	29.236	1.00	4.15	PROT
ATOM	1078	CD2	LEU	360	50.247	6.892	31.432	1.00	18.93	PROT
ATOM	1079	C	LEU	360	51.437	3.001	32.638	1.00	19.29	PROT
ATOM	1080	O	LEU	360	50.319	2.802	33.102	1.00	27.53	PROT
ATOM	1081	N	SER	361	52.375	2.061	32.596	1.00	21.73	PROT
ATOM	1082	CA	SER	361	52.139	0.712	33.114	1.00	23.03	PROT
ATOM	1083	CB	SER	361	53.415	-0.130	33.027	1.00	25.89	PROT
ATOM	1084	OG	SER	361	53.645	-0.613	31.717	1.00	27.77	PROT
ATOM	1085	C	SER	361	51.681	0.730	34.563	1.00	23.26	PROT
ATOM	1086	O	SER	361	50.720	0.046	34.929	1.00	18.73	PROT
ATOM	1087	N	SER	362	52.388	1.524	35.367	1.00	29.84	PROT
ATOM	1088	CA	SER	362	52.141	1.668	36.799	1.00	24.49	PROT
ATOM	1089	CB	SER	362	53.435	2.089	37.491	1.00	26.14	PROT
ATOM	1090	OG	SER	362	53.917	3.305	36.949	1.00	25.03	PROT
ATOM	1091	C	SER	362	51.031	2.635	37.210	1.00	26.86	PROT
ATOM	1092	O	SER	362	50.797	2.831	38.404	1.00	39.63	PROT
ATOM	1093	N	PHE	363	50.361	3.251	36.240	1.00	20.94	PROT
ATOM	1094	CA	PHE	363	49.272	4.185	36.545	1.00	18.33	PROT
ATOM	1095	CB	PHE	363	49.191	5.294	35.486	1.00	17.03	PROT
ATOM	1096	CG	PHE	363	50.171	6.407	35.706	1.00	22.73	PROT
ATOM	1097	CD1	PHE	363	49.733	7.689	35.990	1.00	9.72	PROT
ATOM	1098	CD2	PHE	363	51.545	6.167	35.659	1.00	24.77	PROT
ATOM	1099	CE1	PHE	363	50.645	8.712	36.225	1.00	16.85	PROT
ATOM	1100	CE2	PHE	363	52.463	7.198	35.897	1.00	14.26	PROT
ATOM	1101	CZ	PHE	363	52.011	8.462	36.179	1.00	2.26	PROT
ATOM	1102	C	PHE	363	47.958	3.417	36.598	1.00	16.57	PROT
ATOM	1103	O	PHE	363	46.971	3.882	37.165	1.00	13.08	PROT
ATOM	1104	N	ASN	364	47.976	2.231	36.002	1.00	17.31	PROT
ATOM	1105	CA	ASN	364	46.819	1.349	35.949	1.00	26.11	PROT
ATOM	1106	CB	ASN	364	46.673	0.608	37.276	1.00	16.96	PROT
ATOM	1107	CG	ASN	364	47.402	-0.715	37.267	1.00	31.34	PROT
ATOM	1108	OD1	ASN	364	46.965	-1.657	36.613	1.00	36.66	PROT
ATOM	1109	ND2	ASN	364	48.527	-0.794	37.985	1.00	31.61	PROT
ATOM	1110	C								



ATOM	1114	CB	LEU	365	44.833	4.483	32.861	1.00	16.55	PROT
ATOM	1115	CG	LEU	365	45.762	5.653	33.181	1.00	19.56	PROT
ATOM	1116	CD1	LEU	365	46.146	6.373	31.897	1.00	6.69	PROT
ATOM	1117	CD2	LEU	365	45.067	6.602	34.128	1.00	15.69	PROT
ATOM	1118	C	LEU	365	43.328	2.624	33.520	1.00	12.07	PROT
ATOM	1119	O	LEU	365	43.620	1.534	33.043	1.00	19.81	PROT
ATOM	1120	N	ASP	366	42.077	3.047	33.653	1.00	10.86	PROT
ATOM	1121	CA	ASP	366	40.942	2.263	33.180	1.00	8.96	PROT
ATOM	1122	CB	ASP	366	39.933	2.021	34.326	1.00	9.59	PROT
ATOM	1123	CG	ASP	366	39.300	3.306	34.859	1.00	21.78	PROT
ATOM	1124	OD1	ASP	366	39.871	4.397	34.676	1.00	25.60	PROT
ATOM	1125	OD2	ASP	366	38.217	3.222	35.474	1.00	19.16	PROT
ATOM	1126	C	ASP	366	40.288	3.005	32.002	1.00	8.82	PROT
ATOM	1127	O	ASP	366	40.666	4.132	31.681	1.00	17.66	PROT
ATOM	1128	N	ASP	367	39.321	2.379	31.346	1.00	9.45	PROT
ATOM	1129	CA	ASP	367	38.668	3.023	30.218	1.00	11.11	PROT
ATOM	1130	CB	ASP	367	37.457	2.205	29.769	1.00	20.67	PROT
ATOM	1131	CG	ASP	367	37.832	0.812	29.301	1.00	25.02	PROT
ATOM	1132	OD1	ASP	367	39.040	0.525	29.158	1.00	21.06	PROT
ATOM	1133	OD2	ASP	367	36.909	0.002	29.076	1.00	31.37	PROT
ATOM	1134	C	ASP	367	38.233	4.445	30.574	1.00	14.44	PROT
ATOM	1135	O	ASP	367	38.457	5.380	29.815	1.00	26.42	PROT
ATOM	1136	N	THR	368	37.619	4.612	31.735	1.00	13.62	PROT
ATOM	1137	CA	THR	368	37.157	5.926	32.160	1.00	13.14	PROT
ATOM	1138	CB	THR	368	36.510	5.853	33.547	1.00	16.53	PROT
ATOM	1139	OG1	THR	368	35.482	4.856	33.550	1.00	10.44	PROT
ATOM	1140	CG2	THR	368	35.928	7.188	33.925	1.00	5.20	PROT
ATOM	1141	C	THR	368	38.291	6.942	32.226	1.00	13.03	PROT
ATOM	1142	O	THR	368	38.114	8.108	31.878	1.00	12.90	PROT
ATOM	1143	N	GLU	369	39.455	6.492	32.686	1.00	9.96	PROT
ATOM	1144	CA	GLU	369	40.616	7.365	32.821	1.00	7.34	PROT
ATOM	1145	CB	GLU	369	41.673	6.687	33.708	1.00	10.25	PROT
ATOM	1146	CG	GLU	369	41.584	7.113	35.189	1.00	14.56	PROT
ATOM	1147	CD	GLU	369	41.599	5.945	36.167	1.00	19.39	PROT
ATOM	1148	OE1	GLU	369	42.255	4.922	35.864	1.00	19.65	PROT
ATOM	1149	OE2	GLU	369	40.954	6.054	37.233	1.00	7.98	PROT
ATOM	1150	C	GLU	369	41.203	7.768	31.468	1.00	4.33	PROT
ATOM	1151	O	GLU	369	41.467	8.944	31.213	1.00	7.50	PROT
ATOM	1152	N	VAL	370	41.406	6.784	30.603	1.00	12.29	PROT
ATOM	1153	CA	VAL	370	41.927	7.040	29.267	1.00	19.01	PROT
ATOM	1154	CB	VAL	370	42.092	5.726	28.496	1.00	10.10	PROT
ATOM	1155	CG1	VAL	370	42.431	6.011	27.049	1.00	8.57	PROT
ATOM	1156	CG2								



ATOM	1160	CA	ALA	371	38.549	8.321	28.157	1.00	3.53	PROT
ATOM	1161	CB	ALA	371	37.215	7.728	28.591	1.00	9.17	PROT
ATOM	1162	C	ALA	371	38.603	9.797	28.529	1.00	9.97	PROT
ATOM	1163	O	ALA	371	38.626	10.666	27.655	1.00	24.55	PROT
ATOM	1164	N	LEU	372	38.633	10.082	29.831	1.00	14.85	PROT
ATOM	1165	CA	LEU	372	38.636	11.463	30.307	1.00	9.24	PROT
ATOM	1166	CB	LEU	372	38.480	11.501	31.830	1.00	8.83	PROT
ATOM	1167	CG	LEU	372	37.043	11.288	32.364	1.00	5.50	PROT
ATOM	1168	CD1	LEU	372	37.036	10.338	33.553	1.00	2.02	PROT
ATOM	1169	CD2	LEU	372	36.455	12.626	32.770	1.00	2.00	PROT
ATOM	1170	C	LEU	372	39.867	12.218	29.870	1.00	10.17	PROT
ATOM	1171	O	LEU	372	39.791	13.413	29.568	1.00	7.23	PROT
ATOM	1172	N	LEU	373	40.996	11.510	29.825	1.00	13.10	PROT
ATOM	1173	CA	LEU	373	42.270	12.078	29.399	1.00	2.00	PROT
ATOM	1174	CB	LEU	373	43.325	10.981	29.381	1.00	2.00	PROT
ATOM	1175	CG	LEU	373	44.705	11.118	30.045	1.00	9.64	PROT
ATOM	1176	CD1	LEU	373	44.817	12.382	30.875	1.00	2.00	PROT
ATOM	1177	CD2	LEU	373	44.955	9.883	30.882	1.00	2.00	PROT
ATOM	1178	C	LEU	373	42.026	12.602	27.987	1.00	6.58	PROT
ATOM	1179	O	LEU	373	42.357	13.738	27.660	1.00	9.73	PROT
ATOM	1180	N	GLN	374	41.401	11.763	27.165	1.00	9.45	PROT
ATOM	1181	CA	GLN	374	41.076	12.097	25.785	1.00	2.00	PROT
ATOM	1182	CB	GLN	374	40.382	10.914	25.121	1.00	2.00	PROT
ATOM	1183	CG	GLN	374	41.332	9.896	24.537	1.00	2.00	PROT
ATOM	1184	CD	GLN	374	40.630	8.641	24.095	1.00	2.00	PROT
ATOM	1185	OE1	GLN	374	41.261	7.622	23.855	1.00	8.01	PROT
ATOM	1186	NE2	GLN	374	39.316	8.705	23.989	1.00	2.00	PROT
ATOM	1187	C	GLN	374	40.187	13.326	25.694	1.00	2.78	PROT
ATOM	1188	O	GLN	374	40.427	14.213	24.875	1.00	13.91	PROT
ATOM	1189	N	ALA	375	39.151	13.386	26.521	1.00	2.00	PROT
ATOM	1190	CA	ALA	375	38.261	14.546	26.505	1.00	2.00	PROT
ATOM	1191	CB	ALA	375	37.128	14.348	27.489	1.00	3.97	PROT
ATOM	1192	C	ALA	375	39.061	15.801	26.868	1.00	4.60	PROT
ATOM	1193	O	ALA	375	38.881	16.864	26.274	1.00	8.82	PROT
ATOM	1194	N	VAL	376	39.956	15.667	27.842	1.00	9.01	PROT
ATOM	1195	CA	VAL	376	40.772	16.790	28.267	1.00	7.36	PROT
ATOM	1196	CB	VAL	376	41.669	16.401	29.467	1.00	2.30	PROT
ATOM	1197	CG1	VAL	376	42.597	17.532	29.839	1.00	2.00	PROT
ATOM	1198	CG2	VAL	376	40.801	16.076	30.646	1.00	9.15	PROT
ATOM	1199	C	VAL	376	41.629	17.256	27.110	1.00	3.94	PROT
ATOM	1200	O	VAL	376	41.788	18.455	26.880	1.00	2.00	PROT
ATOM	1201	N	LEU	377	42.179	16.297	26.379	1.00	3.92	PROT
ATOM	1202	CA	LEU	377	43.020	16.618	25.239	1.00	5.65	PROT
ATOM	1203	CB	LEU	377	43.714	15.354	24.731	1.00	5.08	PROT
ATOM	1204	CG	LEU	377	45.052	15.005	25.386	1.00	2.00	PROT
ATOM	1205	CD1	LEU	377	45.620	13.790	24.719	1.00	2.00	PROT

ATOM	1206	CD2	LEU	377	46.016	16.157	25.264	1.00	4.14	PROT
ATOM	1207	C	LEU	377	42.173	17.271	24.137	1.00	11.35	PROT
ATOM	1208	O	LEU	377	42.607	18.240	23.515	1.00	8.78	PROT
ATOM	1209	N	LEU	378	40.959	16.766	23.912	1.00	5.62	PROT
ATOM	1210	CA	LEU	378	40.080	17.352	22.900	1.00	8.57	PROT
ATOM	1211	CB	LEU	378	38.784	16.553	22.788	1.00	5.98	PROT
ATOM	1212	CG	LEU	378	37.847	16.993	21.658	1.00	6.60	PROT
ATOM	1213	CD1	LEU	378	38.550	16.826	20.329	1.00	2.00	PROT
ATOM	1214	CD2	LEU	378	36.563	16.172	21.690	1.00	9.27	PROT
ATOM	1215	C	LEU	378	39.738	18.833	23.146	1.00	10.76	PROT
ATOM	1216	O	LEU	378	40.045	19.689	22.312	1.00	14.81	PROT
ATOM	1217	N	MET	379	39.106	19.139	24.278	1.00	13.15	PROT
ATOM	1218	CA	MET	379	38.735	20.521	24.591	1.00	13.60	PROT
ATOM	1219	CB	MET	379	37.698	20.543	25.709	1.00	12.57	PROT
ATOM	1220	CG	MET	379	36.425	19.782	25.395	1.00	21.12	PROT
ATOM	1221	SD	MET	379	35.533	20.396	23.927	1.00	15.79	PROT
ATOM	1222	CE	MET	379	34.397	19.099	23.756	1.00	13.95	PROT
ATOM	1223	C	MET	379	39.912	21.419	24.988	1.00	16.01	PROT
ATOM	1224	O	MET	379	39.981	21.897	26.121	1.00	16.95	PROT
ATOM	1225	N	SER	380	40.824	21.663	24.048	1.00	12.39	PROT
ATOM	1226	CA	SER	380	41.984	22.506	24.303	1.00	10.77	PROT
ATOM	1227	CB	SER	380	43.248	21.815	23.810	1.00	8.45	PROT
ATOM	1228	OG	SER	380	43.288	20.487	24.286	1.00	17.27	PROT
ATOM	1229	C	SER	380	41.825	23.859	23.621	1.00	15.58	PROT
ATOM	1230	O	SER	380	42.125	24.019	22.432	1.00	23.09	PROT
ATOM	1231	N	SER	381	41.368	24.837	24.396	1.00	23.65	PROT
ATOM	1232	CA	SER	381	41.123	26.187	23.904	1.00	25.18	PROT
ATOM	1233	CB	SER	381	40.449	27.018	25.003	1.00	34.78	PROT
ATOM	1234	OG	SER	381	41.250	27.073	26.170	1.00	37.79	PROT
ATOM	1235	C	SER	381	42.342	26.940	23.388	1.00	19.38	PROT
ATOM	1236	O	SER	381	42.216	28.032	22.850	1.00	28.81	PROT
ATOM	1237	N	ASP	382	43.519	26.361	23.523	1.00	11.80	PROT
ATOM	1238	CA	ASP	382	44.716	27.057	23.082	1.00	15.78	PROT
ATOM	1239	CB	ASP	382	45.908	26.595	23.909	1.00	33.97	PROT
ATOM	1240	CG	ASP	382	46.069	25.098	23.891	1.00	48.78	PROT
ATOM	1241	OD1	ASP	382	45.169	24.401	24.406	1.00	45.58	PROT
ATOM	1242	OD2	ASP	382	47.091	24.620	23.356	1.00	56.52	PROT
ATOM	1243	C	ASP	382	45.037	26.888	21.604	1.00	21.28	PROT
ATOM	1244	O	ASP	382	45.907	27.585	21.079	1.00	41.91	PROT
ATOM	1245	N	ARG	383	44.357	25.971	20.923	1.00	21.81	PROT
ATOM	1246	CA	ARG	383	44.636	25.773	19.503	1.00	18.95	PROT
ATOM	1247	CB	ARG	383	43.745	24.685	18.921	1.00	8.26	

ATOM	1252	NH1	ARG	383	45.187	19.365	21.481	1.00	5.24	PROT
ATOM	1253	NH2	ARG	383	46.717	20.765	20.495	1.00	19.21	PROT
ATOM	1254	C	ARG	383	44.420	27.064	18.728	1.00	19.64	PROT
ATOM	1255	O	ARG	383	43.493	27.828	19.001	1.00	17.46	PROT
ATOM	1256	N	PRO	384	45.298	27.342	17.762	1.00	25.37	PROT
ATOM	1257	CD	PRO	384	46.485	26.567	17.359	1.00	35.06	PROT
ATOM	1258	CA	PRO	384	45.124	28.569	16.983	1.00	27.53	PROT
ATOM	1259	CB	PRO	384	46.422	28.693	16.181	1.00	18.75	PROT
ATOM	1260	CG	PRO	384	47.041	27.338	16.190	1.00	27.78	PROT
ATOM	1261	C	PRO	384	43.895	28.476	16.081	1.00	28.76	PROT
ATOM	1262	O	PRO	384	43.562	27.402	15.560	1.00	31.18	PROT
ATOM	1263	N	GLY	385	43.215	29.606	15.917	1.00	27.37	PROT
ATOM	1264	CA	GLY	385	42.039	29.638	15.073	1.00	26.98	PROT
ATOM	1265	C	GLY	385	40.728	29.442	15.803	1.00	27.46	PROT
ATOM	1266	O	GLY	385	39.689	29.911	15.339	1.00	31.99	PROT
ATOM	1267	N	LEU	386	40.756	28.756	16.939	1.00	34.99	PROT
ATOM	1268	CA	LEU	386	39.524	28.515	17.673	1.00	37.24	PROT
ATOM	1269	CB	LEU	386	39.820	27.947	19.059	1.00	26.60	PROT
ATOM	1270	CG	LEU	386	40.233	26.472	18.988	1.00	32.45	PROT
ATOM	1271	CD1	LEU	386	40.177	25.859	20.363	1.00	34.82	PROT
ATOM	1272	CD2	LEU	386	39.314	25.719	18.030	1.00	29.64	PROT
ATOM	1273	C	LEU	386	38.733	29.795	17.778	1.00	36.93	PROT
ATOM	1274	O	LEU	386	39.291	30.881	17.674	1.00	37.60	PROT
ATOM	1275	N	ALA	387	37.427	29.665	17.962	1.00	31.47	PROT
ATOM	1276	CA	ALA	387	36.578	30.832	18.058	1.00	28.80	PROT
ATOM	1277	CB	ALA	387	35.553	30.814	16.950	1.00	41.01	PROT
ATOM	1278	C	ALA	387	35.890	30.864	19.400	1.00	28.89	PROT
ATOM	1279	O	ALA	387	35.998	31.842	20.133	1.00	30.62	PROT
ATOM	1280	N	CYS	388	35.167	29.797	19.710	1.00	25.92	PROT
ATOM	1281	CA	CYS	388	34.469	29.712	20.978	1.00	26.90	PROT
ATOM	1282	CB	CYS	388	33.224	28.823	20.826	1.00	21.38	PROT
ATOM	1283	SG	CYS	388	31.625	29.732	20.698	1.00	33.66	PROT
ATOM	1284	C	CYS	388	35.443	29.159	22.040	1.00	31.18	PROT
ATOM	1285	O	CYS	388	35.272	28.054	22.552	1.00	36.57	PROT
ATOM	1286	N	VAL	389	36.473	29.951	22.346	1.00	20.22	PROT
ATOM	1287	CA	VAL	389	37.511	29.622	23.327	1.00	16.02	PROT
ATOM	1288	CB	VAL	389	38.554	30.737	23.381	1.00	9.80	PROT
ATOM	1289	CG1	VAL	389	39.526	30.480	24.498	1.00	16.03	PROT
ATOM	1290	CG2	VAL	389	39.257	30.843	22.056	1.00	16.27	PROT
ATOM	1291	C	VAL	389	36.977	29.425	24.753	1.00	18.85	PROT
ATOM	1292	O	VAL	389	37.066	28.336	25.323	1.00	24.21	PROT
ATOM	1293	N	GLU	390	36.461	30.500	25.337	1.00		

ATOM	1298	N	ARG	391	34.103	28.938	25.915	1.00	14.06	PROT
ATOM	1299	CA	ARG	391	33.248	27.754	26.093	1.00	26.18	PROT
ATOM	1300	CB	ARG	391	32.121	27.699	25.049	1.00	31.84	PROT
ATOM	1301	CG	ARG	391	30.843	27.040	25.601	1.00	47.73	PROT
ATOM	1302	CD	ARG	391	29.882	26.572	24.512	1.00	58.24	PROT
ATOM	1303	NE	ARG	391	29.879	27.487	23.378	1.00	66.80	PROT
ATOM	1304	CZ	ARG	391	29.001	28.470	23.211	1.00	69.56	PROT
ATOM	1305	NH1	ARG	391	29.088	29.255	22.139	1.00	66.99	PROT
ATOM	1306	NH2	ARG	391	28.034	28.663	24.105	1.00	56.08	PROT
ATOM	1307	C	ARG	391	33.979	26.415	26.110	1.00	23.65	PROT
ATOM	1308	O	ARG	391	33.561	25.479	26.794	1.00	28.58	PROT
ATOM	1309	N	ILE	392	35.064	26.316	25.359	1.00	15.05	PROT
ATOM	1310	CA	ILE	392	35.812	25.077	25.335	1.00	19.03	PROT
ATOM	1311	CB	ILE	392	36.804	25.063	24.165	1.00	22.30	PROT
ATOM	1312	CG2	ILE	392	37.971	24.130	24.467	1.00	21.71	PROT
ATOM	1313	CG1	ILE	392	36.074	24.614	22.892	1.00	23.47	PROT
ATOM	1314	CD1	ILE	392	36.245	25.551	21.707	1.00	4.13	PROT
ATOM	1315	C	ILE	392	36.544	24.907	26.671	1.00	25.03	PROT
ATOM	1316	O	ILE	392	36.728	23.783	27.153	1.00	26.11	PROT
ATOM	1317	N	GLU	393	36.947	26.029	27.266	1.00	30.74	PROT
ATOM	1318	CA	GLU	393	37.630	26.021	28.558	1.00	23.39	PROT
ATOM	1319	CB	GLU	393	38.073	27.430	28.930	1.00	27.18	PROT
ATOM	1320	CG	GLU	393	39.435	27.817	28.402	1.00	41.39	PROT
ATOM	1321	CD	GLU	393	39.990	29.051	29.093	1.00	47.72	PROT
ATOM	1322	OE1	GLU	393	39.365	29.524	30.070	1.00	39.94	PROT
ATOM	1323	OE2	GLU	393	41.051	29.547	28.653	1.00	51.17	PROT
ATOM	1324	C	GLU	393	36.655	25.516	29.610	1.00	21.72	PROT
ATOM	1325	O	GLU	393	36.942	24.574	30.344	1.00	22.82	PROT
ATOM	1326	N	LYS	394	35.497	26.163	29.676	1.00	9.64	PROT
ATOM	1327	CA	LYS	394	34.462	25.779	30.618	1.00	11.56	PROT
ATOM	1328	CB	LYS	394	33.177	26.557	30.338	1.00	7.52	PROT
ATOM	1329	C	LYS	394	34.213	24.280	30.492	1.00	16.31	PROT
ATOM	1330	O	LYS	394	34.000	23.594	31.498	1.00	24.52	PROT
ATOM	1331	N	TYR	395	34.251	23.763	29.264	1.00	12.79	PROT
ATOM	1332	CA	TYR	395	34.033	22.332	29.057	1.00	19.02	PROT
ATOM	1333	CB	TYR	395	33.803	22.025	27.572	1.00	27.90	PROT
ATOM	1334	CG	TYR	395	32.454	22.456	27.027	1.00	31.64	PROT
ATOM	1335	CD1	TYR	395	32.136	22.267	25.684	1.00	30.15	PROT
ATOM	1336	CE1	TYR	395	30.927	22.695	25.160	1.00	28.34	PROT
ATOM	1337	CD2	TYR	395	31.514	23.085	27.835	1.00	34.21	PROT
ATOM	1338	CE2	TYR	395	30.298	23.518	27.317	1.00	34.01	PROT
ATOM	1339	CZ	TYR	395	30.014	23.322				



ATOM	1344	CA	GLN	396	37.596	21.134	29.725	1.00	13.73	PROT
ATOM	1345	CB	GLN	396	38.905	21.766	29.240	1.00	2.45	PROT
ATOM	1346	CG	GLN	396	40.061	20.767	29.110	1.00	2.00	PROT
ATOM	1347	CD	GLN	396	41.388	21.439	28.799	1.00	5.12	PROT
ATOM	1348	OE1	GLN	396	41.706	22.484	29.359	1.00	10.11	PROT
ATOM	1349	NE2	GLN	396	42.169	20.840	27.903	1.00	9.09	PROT
ATOM	1350	C	GLN	396	37.562	21.149	31.238	1.00	17.65	PROT
ATOM	1351	O	GLN	396	37.802	20.125	31.894	1.00	9.63	PROT
ATOM	1352	N	ASP	397	37.250	22.319	31.787	1.00	6.69	PROT
ATOM	1353	CA	ASP	397	37.178	22.476	33.226	1.00	9.36	PROT
ATOM	1354	CB	ASP	397	36.732	23.893	33.570	1.00	11.44	PROT
ATOM	1355	CG	ASP	397	37.867	24.891	33.446	1.00	18.32	PROT
ATOM	1356	OD1	ASP	397	39.033	24.438	33.397	1.00	24.00	PROT
ATOM	1357	OD2	ASP	397	37.615	26.114	33.395	1.00	20.67	PROT
ATOM	1358	C	ASP	397	36.215	21.443	33.771	1.00	7.77	PROT
ATOM	1359	O	ASP	397	36.497	20.771	34.761	1.00	7.66	PROT
ATOM	1360	N	SER	398	35.087	21.293	33.093	1.00	9.19	PROT
ATOM	1361	CA	SER	398	34.094	20.322	33.508	1.00	14.18	PROT
ATOM	1362	CB	SER	398	32.916	20.334	32.542	1.00	12.11	PROT
ATOM	1363	OG	SER	398	32.406	21.650	32.423	1.00	31.95	PROT
ATOM	1364	C	SER	398	34.712	18.939	33.556	1.00	11.47	PROT
ATOM	1365	O	SER	398	34.591	18.227	34.551	1.00	21.11	PROT
ATOM	1366	N	PHE	399	35.394	18.565	32.485	1.00	18.68	PROT
ATOM	1367	CA	PHE	399	36.017	17.252	32.417	1.00	24.93	PROT
ATOM	1368	CB	PHE	399	36.587	17.012	31.014	1.00	23.38	PROT
ATOM	1369	CG	PHE	399	35.543	16.705	29.981	1.00	20.19	PROT
ATOM	1370	CD1	PHE	399	35.224	17.638	28.997	1.00	22.94	PROT
ATOM	1371	CD2	PHE	399	34.878	15.486	29.988	1.00	8.62	PROT
ATOM	1372	CE1	PHE	399	34.257	17.361	28.029	1.00	12.53	PROT
ATOM	1373	CE2	PHE	399	33.914	15.201	29.027	1.00	19.25	PROT
ATOM	1374	CZ	PHE	399	33.604	16.143	28.044	1.00	15.15	PROT
ATOM	1375	C	PHE	399	37.113	17.097	33.463	1.00	23.06	PROT
ATOM	1376	O	PHE	399	37.210	16.063	34.137	1.00	15.58	PROT
ATOM	1377	N	LEU	400	37.932	18.131	33.604	1.00	22.12	PROT
ATOM	1378	CA	LEU	400	39.017	18.095	34.567	1.00	18.27	PROT
ATOM	1379	CB	LEU	400	39.846	19.372	34.461	1.00	10.06	PROT
ATOM	1380	CG	LEU	400	41.021	19.248	33.491	1.00	8.13	PROT
ATOM	1381	CD1	LEU	400	41.616	20.594	33.195	1.00	2.00	PROT
ATOM	1382	CD2	LEU	400	42.055	18.333	34.095	1.00	13.73	PROT
ATOM	1383	C	LEU	400	38.527	17.892	36.002	1.00	24.79	PROT
ATOM	1384	O	LEU	400	39.189	17.228	36.787	1.00	26.46	PROT
ATOM	1385	N	LEU	401	37.371	18.447	36.354	1.00</		



ATOM	1390	CD2	LEU	401	34.206	20.235	39.687	1.00	14.41	PROT
ATOM	1391	C	LEU	401	36.316	16.864	37.879	1.00	18.03	PROT
ATOM	1392	O	LEU	401	36.482	16.250	38.925	1.00	28.63	PROT
ATOM	1393	N	ALA	402	35.656	16.346	36.856	1.00	9.30	PROT
ATOM	1394	CA	ALA	402	35.124	15.000	36.951	1.00	7.03	PROT
ATOM	1395	CB	ALA	402	34.233	14.703	35.758	1.00	14.15	PROT
ATOM	1396	C	ALA	402	36.298	14.029	36.989	1.00	7.68	PROT
ATOM	1397	O	ALA	402	36.294	13.054	37.739	1.00	2.00	PROT
ATOM	1398	N	PHE	403	37.311	14.305	36.178	1.00	4.49	PROT
ATOM	1399	CA	PHE	403	38.477	13.439	36.140	1.00	9.18	PROT
ATOM	1400	CB	PHE	403	39.510	13.977	35.138	1.00	12.80	PROT
ATOM	1401	CG	PHE	403	40.545	12.957	34.693	1.00	5.42	PROT
ATOM	1402	CD1	PHE	403	41.590	13.334	33.859	1.00	2.00	PROT
ATOM	1403	CD2	PHE	403	40.480	11.634	35.103	1.00	2.00	PROT
ATOM	1404	CE1	PHE	403	42.546	12.410	33.448	1.00	2.00	PROT
ATOM	1405	CE2	PHE	403	41.440	10.711	34.688	1.00	2.00	PROT
ATOM	1406	CZ	PHE	403	42.468	11.100	33.863	1.00	2.00	PROT
ATOM	1407	C	PHE	403	39.080	13.366	37.539	1.00	10.08	PROT
ATOM	1408	O	PHE	403	39.207	12.279	38.097	1.00	8.23	PROT
ATOM	1409	N	GLU	404	39.451	14.514	38.103	1.00	12.64	PROT
ATOM	1410	CA	GLU	404	40.030	14.546	39.448	1.00	19.23	PROT
ATOM	1411	CB	GLU	404	40.227	15.989	39.942	1.00	19.80	PROT
ATOM	1412	CG	GLU	404	41.532	16.220	40.728	1.00	24.03	PROT
ATOM	1413	CD	GLU	404	41.474	17.429	41.655	1.00	29.60	PROT
ATOM	1414	OE1	GLU	404	41.706	18.565	41.182	1.00	29.51	PROT
ATOM	1415	OE2	GLU	404	41.197	17.247	42.861	1.00	30.42	PROT
ATOM	1416	C	GLU	404	39.112	13.806	40.416	1.00	24.36	PROT
ATOM	1417	O	GLU	404	39.571	12.963	41.200	1.00	28.04	PROT
ATOM	1418	N	HIS	405	37.815	14.108	40.358	1.00	10.26	PROT
ATOM	1419	CA	HIS	405	36.870	13.446	41.240	1.00	7.78	PROT
ATOM	1420	CB	HIS	405	35.473	14.023	41.054	1.00	3.47	PROT
ATOM	1421	CG	HIS	405	35.312	15.393	41.630	1.00	15.49	PROT
ATOM	1422	CD2	HIS	405	36.223	16.260	42.134	1.00	17.97	PROT
ATOM	1423	ND1	HIS	405	34.096	16.036	41.694	1.00	21.57	PROT
ATOM	1424	CE1	HIS	405	34.265	17.242	42.210	1.00	27.50	PROT
ATOM	1425	NE2	HIS	405	35.547	17.403	42.485	1.00	13.53	PROT
ATOM	1426	C	HIS	405	36.856	11.936	41.005	1.00	14.88	PROT
ATOM	1427	O	HIS	405	36.641	11.155	41.935	1.00	22.11	PROT
ATOM	1428	N	TYR	406	37.091	11.512	39.767	1.00	16.52	PROT
ATOM	1429	CA	TYR	406	37.085	10.083	39.491	1.00	14.35	PROT
ATOM	1430	CB	TYR	406	37.007	9.808	37.989	1.00	9.90	PROT
ATOM	1431	CG	TYR	406	36.840	8.346	37.657	1.00	2	

ATOM	1436	CZ	TYR	406	36.548	5.624	37.073	1.00	15.64	PROT
ATOM	1437	OH	TYR	406	36.431	4.287	36.804	1.00	2.00	PROT
ATOM	1438	C	TYR	406	38.340	9.466	40.071	1.00	9.54	PROT
ATOM	1439	O	TYR	406	38.328	8.328	40.525	1.00	14.29	PROT
ATOM	1440	N	ILE	407	39.430	10.217	40.058	1.00	6.56	PROT
ATOM	1441	CA	ILE	407	40.671	9.708	40.617	1.00	13.87	PROT
ATOM	1442	CB	ILE	407	41.808	10.728	40.474	1.00	11.28	PROT
ATOM	1443	CG2	ILE	407	42.902	10.413	41.461	1.00	6.25	PROT
ATOM	1444	CG1	ILE	407	42.357	10.714	39.039	1.00	18.73	PROT
ATOM	1445	CD1	ILE	407	41.863	9.579	38.169	1.00	13.14	PROT
ATOM	1446	C	ILE	407	40.438	9.426	42.091	1.00	11.44	PROT
ATOM	1447	O	ILE	407	40.691	8.325	42.571	1.00	4.46	PROT
ATOM	1448	N	ASN	408	39.953	10.448	42.792	1.00	12.35	PROT
ATOM	1449	CA	ASN	408	39.642	10.363	44.213	1.00	2.00	PROT
ATOM	1450	CB	ASN	408	38.758	11.535	44.629	1.00	2.00	PROT
ATOM	1451	CG	ASN	408	39.499	12.840	44.657	1.00	3.57	PROT
ATOM	1452	OD1	ASN	408	40.733	12.859	44.656	1.00	14.35	PROT
ATOM	1453	ND2	ASN	408	38.758	13.949	44.689	1.00	2.00	PROT
ATOM	1454	C	ASN	408	38.868	9.078	44.432	1.00	6.49	PROT
ATOM	1455	O	ASN	408	39.282	8.187	45.178	1.00	10.45	PROT
ATOM	1456	N	TYR	409	37.731	8.987	43.766	1.00	2.00	PROT
ATOM	1457	CA	TYR	409	36.900	7.816	43.893	1.00	9.20	PROT
ATOM	1458	CB	TYR	409	35.879	7.783	42.760	1.00	11.66	PROT
ATOM	1459	CG	TYR	409	35.121	6.489	42.683	1.00	12.54	PROT
ATOM	1460	CD1	TYR	409	33.984	6.281	43.456	1.00	29.23	PROT
ATOM	1461	CE1	TYR	409	33.285	5.077	43.403	1.00	25.45	PROT
ATOM	1462	CD2	TYR	409	35.547	5.465	41.850	1.00	24.96	PROT
ATOM	1463	CE2	TYR	409	34.860	4.259	41.788	1.00	33.40	PROT
ATOM	1464	CZ	TYR	409	33.733	4.074	42.567	1.00	24.27	PROT
ATOM	1465	OH	TYR	409	33.065	2.883	42.509	1.00	32.72	PROT
ATOM	1466	C	TYR	409	37.753	6.553	43.867	1.00	13.96	PROT
ATOM	1467	O	TYR	409	37.730	5.763	44.804	1.00	29.48	PROT
ATOM	1468	N	ARG	410	38.531	6.399	42.803	1.00	23.04	PROT
ATOM	1469	CA	ARG	410	39.377	5.230	42.588	1.00	22.09	PROT
ATOM	1470	CB	ARG	410	39.982	5.327	41.190	1.00	13.24	PROT
ATOM	1471	CG	ARG	410	38.947	5.399	40.090	1.00	14.01	PROT
ATOM	1472	CD	ARG	410	38.934	4.111	39.275	1.00	16.49	PROT
ATOM	1473	NE	ARG	410	40.227	3.848	38.651	1.00	9.77	PROT
ATOM	1474	CZ	ARG	410	40.617	2.651	38.239	1.00	11.38	PROT
ATOM	1475	NH1	ARG	410	41.806	2.493	37.685	1.00	14.94	PROT
ATOM	1476	NH2	ARG	410	39.810	1.613	38.375	1.00	12.78	PROT
ATOM	1477	C	ARG	410	40.486	4.914	43.604	1.00	24.49	PROT
ATOM										

ATOM	1482	CG	LYS	411	40.317	5.779	47.103	1.00	35.00	PROT
ATOM	1483	CD	LYS	411	39.406	4.788	47.804	1.00	40.83	PROT
ATOM	1484	CE	LYS	411	38.414	5.496	48.725	1.00	58.04	PROT
ATOM	1485	NZ	LYS	411	38.833	5.496	50.168	1.00	54.40	PROT
ATOM	1486	C	LYS	411	43.186	4.814	44.664	1.00	28.02	PROT
ATOM	1487	O	LYS	411	43.209	3.598	44.876	1.00	25.00	PROT
ATOM	1488	N	HIS	412	44.091	5.438	43.923	1.00	30.05	PROT
ATOM	1489	CA	HIS	412	45.223	4.738	43.332	1.00	26.70	PROT
ATOM	1490	CB	HIS	412	45.756	5.491	42.104	1.00	29.28	PROT
ATOM	1491	CG	HIS	412	44.953	5.289	40.857	1.00	18.44	PROT
ATOM	1492	CD2	HIS	412	43.783	5.836	40.451	1.00	19.98	PROT
ATOM	1493	ND1	HIS	412	45.366	4.465	39.833	1.00	16.33	PROT
ATOM	1494	CE1	HIS	412	44.486	4.513	38.850	1.00	24.80	PROT
ATOM	1495	NE2	HIS	412	43.516	5.338	39.200	1.00	23.01	PROT
ATOM	1496	C	HIS	412	46.281	4.788	44.406	1.00	20.73	PROT
ATOM	1497	O	HIS	412	46.335	5.740	45.171	1.00	24.69	PROT
ATOM	1498	N	HIS	413	47.138	3.784	44.461	1.00	28.17	PROT
ATOM	1499	CA	HIS	413	48.183	3.788	45.465	1.00	28.09	PROT
ATOM	1500	CB	HIS	413	48.219	2.426	46.144	1.00	21.71	PROT
ATOM	1501	CG	HIS	413	46.906	2.053	46.759	1.00	44.26	PROT
ATOM	1502	CD2	HIS	413	46.140	0.941	46.632	1.00	43.48	PROT
ATOM	1503	ND1	HIS	413	46.214	2.902	47.600	1.00	40.00	PROT
ATOM	1504	CE1	HIS	413	45.080	2.328	47.962	1.00	47.35	PROT
ATOM	1505	NE2	HIS	413	45.011	1.137	47.390	1.00	35.50	PROT
ATOM	1506	C	HIS	413	49.527	4.194	44.875	1.00	26.49	PROT
ATOM	1507	O	HIS	413	50.483	3.421	44.829	1.00	31.82	PROT
ATOM	1508	N	VAL	414	49.555	5.439	44.411	1.00	18.32	PROT
ATOM	1509	CA	VAL	414	50.726	6.069	43.820	1.00	22.60	PROT
ATOM	1510	CB	VAL	414	50.718	5.966	42.290	1.00	32.50	PROT
ATOM	1511	CG1	VAL	414	51.636	7.026	41.694	1.00	33.83	PROT
ATOM	1512	CG2	VAL	414	51.169	4.574	41.863	1.00	40.20	PROT
ATOM	1513	C	VAL	414	50.630	7.529	44.225	1.00	17.96	PROT
ATOM	1514	O	VAL	414	49.708	8.236	43.829	1.00	30.33	PROT
ATOM	1515	N	THR	415	51.586	7.969	45.028	1.00	32.51	PROT
ATOM	1516	CA	THR	415	51.601	9.332	45.531	1.00	35.31	PROT
ATOM	1517	CB	THR	415	52.779	9.529	46.511	1.00	49.75	PROT
ATOM	1518	OG1	THR	415	53.023	10.930	46.702	1.00	60.64	PROT
ATOM	1519	CG2	THR	415	54.038	8.850	45.974	1.00	50.83	PROT
ATOM	1520	C	THR	415	51.668	10.387	44.436	1.00	31.44	PROT
ATOM	1521	O	THR	415	52.423	10.251	43.475	1.00	22.01	PROT
ATOM	1522	N	HIS	416	50.865	11.437	44.607	1.00	24.94	PROT
ATOM	1523	CA	HIS	416	50.781	12.559	43.671	1.00	27.82	PROT
ATOM	15									





ATOM	1574	CA	LEU	421	48.627	12.614	35.297	1.00	9.38	PROT
ATOM	1575	CB	LEU	421	47.231	12.139	35.707	1.00	13.22	PROT
ATOM	1576	CG	LEU	421	46.739	10.818	35.107	1.00	15.75	PROT
ATOM	1577	CD1	LEU	421	47.919	9.993	34.652	1.00	29.24	PROT
ATOM	1578	CD2	LEU	421	45.949	10.049	36.135	1.00	12.19	PROT
ATOM	1579	C-	LEU	421	48.511	13.866	34.441	1.00	12.61	PROT
ATOM	1580	O	LEU	421	48.458	13.777	33.223	1.00	17.85	PROT
ATOM	1581	N	LEU	422	48.451	15.036	35.063	1.00	8.47	PROT
ATOM	1582	CA	LEU	422	48.393	16.254	34.277	1.00	7.21	PROT
ATOM	1583	CB	LEU	422	48.160	17.468	35.164	1.00	2.00	PROT
ATOM	1584	CG	LEU	422	46.941	17.445	36.088	1.00	12.16	PROT
ATOM	1585	CD1	LEU	422	47.024	18.660	36.982	1.00	6.96	PROT
ATOM	1586	CD2	LEU	422	45.632	17.450	35.313	1.00	2.00	PROT
ATOM	1587	C	LEU	422	49.748	16.365	33.567	1.00	10.59	PROT
ATOM	1588	O	LEU	422	49.851	16.938	32.477	1.00	13.48	PROT
ATOM	1589	N	MET	423	50.786	15.804	34.185	1.00	2.29	PROT
ATOM	1590	CA	MET	423	52.109	15.821	33.579	1.00	6.50	PROT
ATOM	1591	CB	MET	423	53.158	15.215	34.514	1.00	2.13	PROT
ATOM	1592	CG	MET	423	53.361	15.968	35.803	1.00	16.33	PROT
ATOM	1593	SD	MET	423	55.075	16.415	36.070	1.00	26.66	PROT
ATOM	1594	CE	MET	423	55.751	14.880	36.623	1.00	20.24	PROT
ATOM	1595	C	MET	423	52.016	14.966	32.318	1.00	12.20	PROT
ATOM	1596	O	MET	423	52.741	15.183	31.345	1.00	18.67	PROT
ATOM	1597	N	LYS	424	51.114	13.988	32.352	1.00	7.89	PROT
ATOM	1598	CA	LYS	424	50.907	13.084	31.230	1.00	12.91	PROT
ATOM	1599	CB	LYS	424	49.990	11.924	31.645	1.00	5.14	PROT
ATOM	1600	CG	LYS	424	50.669	10.579	31.980	1.00	11.76	PROT
ATOM	1601	CD	LYS	424	52.187	10.590	31.866	1.00	3.70	PROT
ATOM	1602	CE	LYS	424	52.844	10.020	33.113	1.00	7.84	PROT
ATOM	1603	NZ	LYS	424	54.335	9.959	32.995	1.00	25.86	PROT
ATOM	1604	C	LYS	424	50.293	13.840	30.046	1.00	17.44	PROT
ATOM	1605	O	LYS	424	50.650	13.596	28.897	1.00	11.72	PROT
ATOM	1606	N	VAL	425	49.370	14.756	30.322	1.00	3.16	PROT
ATOM	1607	CA	VAL	425	48.768	15.515	29.249	1.00	2.00	PROT
ATOM	1608	CB	VAL	425	47.744	16.532	29.773	1.00	6.77	PROT
ATOM	1609	CG1	VAL	425	47.653	17.716	28.815	1.00	2.00	PROT
ATOM	1610	CG2	VAL	425	46.381	15.870	29.914	1.00	10.91	PROT
ATOM	1611	C	VAL	425	49.845	16.274	28.487	1.00	4.83	PROT
ATOM	1612	O	VAL	425	49.853	16.265	27.269	1.00	15.69	PROT
ATOM	1613	N	THR	426	50.753	16.924	29.208	1.00	14.38	PROT
ATOM	1614	CA	THR	426	51.824	17.707	28.593	1.00	12.41	PROT
ATOM	1615	CB	THR	426	52.713	18.372	29.667	1.00	12.49	PROT
ATOM	1616	OG1	THR	426	51.890	19.138	30.552	1.00	11.06	PROT
ATOM	1617	CG2	THR	426	53.763	19.283	29.015	1.00	2.93	PROT
ATOM	1618	C	THR	426	52.734	16.928	27.653	1.00	15.72	PROT
ATOM	1619	O	THR	426	53.198	17.463	26.651	1.00	14.40	PROT



ATOM	1620	N	ASP	427	53.000	15.672	27.981	1.00	16.23	PROT
ATOM	1621	CA	ASP	427	53.865	14.843	27.157	1.00	16.35	PROT
ATOM	1622	CB	ASP	427	54.342	13.630	27.950	1.00	19.48	PROT
ATOM	1623	CG	ASP	427	55.337	13.997	29.029	1.00	18.96	PROT
ATOM	1624	OD1	ASP	427	55.874	15.125	29.010	1.00	8.75	PROT
ATOM	1625	OD2	ASP	427	55.579	13.145	29.902	1.00	24.25	PROT
ATOM	1626	C	ASP	427	53.155	14.381	25.891	1.00	20.52	PROT
ATOM	1627	O	ASP	427	53.793	14.164	24.856	1.00	25.69	PROT
ATOM	1628	N	LEU	428	51.838	14.218	25.986	1.00	5.49	PROT
ATOM	1629	CA	LEU	428	51.040	13.815	24.849	1.00	2.00	PROT
ATOM	1630	CB	LEU	428	49.634	13.470	25.301	1.00	2.00	PROT
ATOM	1631	CG	LEU	428	49.579	12.127	26.028	1.00	2.00	PROT
ATOM	1632	CD1	LEU	428	48.184	11.789	26.481	1.00	2.00	PROT
ATOM	1633	CD2	LEU	428	50.088	11.080	25.108	1.00	2.00	PROT
ATOM	1634	C	LEU	428	51.019	14.987	23.881	1.00	7.72	PROT
ATOM	1635	O	LEU	428	51.072	14.800	22.666	1.00	9.22	PROT
ATOM	1636	N	ARG	429	50.961	16.197	24.432	1.00	10.07	PROT
ATOM	1637	CA	ARG	429	50.948	17.438	23.659	1.00	7.97	PROT
ATOM	1638	CB	ARG	429	50.799	18.642	24.583	1.00	18.55	PROT
ATOM	1639	CG	ARG	429	49.548	18.634	25.429	1.00	14.80	PROT
ATOM	1640	CD	ARG	429	48.588	19.674	24.935	1.00	32.08	PROT
ATOM	1641	NE	ARG	429	47.508	19.923	25.880	1.00	42.46	PROT
ATOM	1642	CZ	ARG	429	46.226	19.673	25.631	1.00	48.51	PROT
ATOM	1643	NH1	ARG	429	45.860	19.163	24.459	1.00	33.35	PROT
ATOM	1644	NH2	ARG	429	45.307	19.955	26.549	1.00	46.08	PROT
ATOM	1645	C	ARG	429	52.260	17.557	22.919	1.00	11.77	PROT
ATOM	1646	O	ARG	429	52.298	17.904	21.737	1.00	28.66	PROT
ATOM	1647	N	MET	430	53.343	17.270	23.629	1.00	20.26	PROT
ATOM	1648	CA	MET	430	54.671	17.328	23.042	1.00	21.06	PROT
ATOM	1649	CB	MET	430	55.738	17.015	24.100	1.00	30.24	PROT
ATOM	1650	CG	MET	430	56.061	18.165	25.056	1.00	34.66	PROT
ATOM	1651	SD	MET	430	55.727	19.795	24.373	1.00	35.91	PROT
ATOM	1652	CE	MET	430	56.839	19.814	22.978	1.00	32.52	PROT
ATOM	1653	C	MET	430	54.735	16.302	21.925	1.00	18.70	PROT
ATOM	1654	O	MET	430	55.287	16.560	20.860	1.00	16.59	PROT
ATOM	1655	N	ILE	431	54.161	15.133	22.182	1.00	15.38	PROT
ATOM	1656	CA	ILE	431	54.144	14.069	21.196	1.00	15.85	PROT
ATOM	1657	CB	ILE	431	53.326	12.859	21.705	1.00	13.76	PROT
ATOM	1658	CG2	ILE	431	52.727	12.084	20.539	1.00	11.11	PROT
ATOM	1659	CG1	ILE	431	54.239	11.924	22.489	1.00	11.72	PROT
ATOM	1660	CD1	ILE	431	53.552	11.224	23.615	1.00	16.22	PROT
ATOM	1661	C	ILE	431	53.538	14.609	19.904	1.00	18	

ATOM	1666	O	GLY	432	52.707	16.834	16.936	1.00	9.60	PROT
ATOM	1667	N	ALA	433	53.043	17.805	18.926	1.00	11.17	PROT
ATOM	1668	CA	ALA	433	53.855	18.884	18.385	1.00	2.00	PROT
ATOM	1669	CB	ALA	433	54.326	19.771	19.506	1.00	2.00	PROT
ATOM	1670	C	ALA	433	55.050	18.285	17.646	1.00	6.43	PROT
ATOM	1671	O-	ALA	433	55.493	18.789	16.623	1.00	11.71	PROT
ATOM	1672	N	CYS	434	55.579	17.197	18.179	1.00	15.71	PROT
ATOM	1673	CA	CYS	434	56.715	16.534	17.573	1.00	13.44	PROT
ATOM	1674	CB	CYS	434	57.228	15.464	18.518	1.00	14.76	PROT
ATOM	1675	SG	CYS	434	58.910	15.703	18.985	1.00	20.82	PROT
ATOM	1676	C	CYS	434	56.269	15.902	16.264	1.00	9.28	PROT
ATOM	1677	O	CYS	434	56.969	15.948	15.256	1.00	8.50	PROT
ATOM	1678	N	HIS	435	55.091	15.300	16.298	1.00	11.04	PROT
ATOM	1679	CA	HIS	435	54.533	14.657	15.122	1.00	11.30	PROT
ATOM	1680	CB	HIS	435	53.142	14.132	15.438	1.00	4.30	PROT
ATOM	1681	CG	HIS	435	52.480	13.460	14.283	1.00	13.68	PROT
ATOM	1682	CD2	HIS	435	52.751	12.288	13.662	1.00	4.72	PROT
ATOM	1683	ND1	HIS	435	51.358	13.976	13.666	1.00	5.53	PROT
ATOM	1684	CE1	HIS	435	50.966	13.147	12.717	1.00	12.84	PROT
ATOM	1685	NE2	HIS	435	51.794	12.116	12.694	1.00	15.77	PROT
ATOM	1686	C	HIS	435	54.482	15.661	13.973	1.00	8.50	PROT
ATOM	1687	O	HIS	435	54.941	15.370	12.869	1.00	14.82	PROT
ATOM	1688	N	ALA	436	53.938	16.844	14.245	1.00	5.74	PROT
ATOM	1689	CA	ALA	436	53.843	17.905	13.252	1.00	2.00	PROT
ATOM	1690	CB	ALA	436	53.632	19.241	13.942	1.00	2.00	PROT
ATOM	1691	C	ALA	436	55.121	17.934	12.406	1.00	8.68	PROT
ATOM	1692	O	ALA	436	55.080	17.712	11.193	1.00	15.14	PROT
ATOM	1693	N	SER	437	56.256	18.189	13.047	1.00	6.82	PROT
ATOM	1694	CA	SER	437	57.522	18.226	12.337	1.00	9.05	PROT
ATOM	1695	CB	SER	437	58.671	18.511	13.295	1.00	2.00	PROT
ATOM	1696	OG	SER	437	59.593	19.406	12.699	1.00	21.18	PROT
ATOM	1697	C	SER	437	57.758	16.896	11.637	1.00	15.18	PROT
ATOM	1698	O	SER	437	58.076	16.849	10.445	1.00	19.33	PROT
ATOM	1699	N	ARG	438	57.607	15.805	12.373	1.00	16.98	PROT
ATOM	1700	CA	ARG	438	57.799	14.501	11.766	1.00	16.98	PROT
ATOM	1701	CB	ARG	438	57.294	13.409	12.702	1.00	24.77	PROT
ATOM	1702	CG	ARG	438	58.006	12.086	12.534	1.00	33.76	PROT
ATOM	1703	CD	ARG	438	59.506	12.280	12.614	1.00	30.64	PROT
ATOM	1704	NE	ARG	438	60.219	11.380	11.721	1.00	29.76	PROT
ATOM	1705	CZ	ARG	438	61.505	11.504	11.423	1.00	25.21	PROT
ATOM	1706	NH1	ARG	438	62.077	10.641	10.603	1.00	39.58	PROT
ATOM	1707	NH2	ARG	438	62.217	12.492	11.942	1.00	14.13	PROT
ATOM										

ATOM	1712	CB	PHE	439	53.603	15.575	9.574	1.00	17.84	PROT
ATOM	1713	CG	PHE	439	52.597	15.364	8.490	1.00	20.60	PROT
ATOM	1714	CD1	PHE	439	52.042	14.103	8.279	1.00	30.60	PROT
ATOM	1715	CD2	PHE	439	52.265	16.394	7.622	1.00	14.95	PROT
ATOM	1716	CE1	PHE	439	51.175	13.867	7.206	1.00	29.12	PROT
ATOM	1717	CE2	PHE	439	51.404	16.173	6.552	1.00	25.18	PROT
ATOM	1718	CZ	PHE	439	50.860	14.905	6.341	1.00	27.82	PROT
ATOM	1719	C	PHE	439	55.620	15.548	8.130	1.00	28.17	PROT
ATOM	1720	O	PHE	439	55.512	15.095	6.987	1.00	28.83	PROT
ATOM	1721	N	LEU	440	56.328	16.633	8.427	1.00	26.77	PROT
ATOM	1722	CA	LEU	440	57.055	17.382	7.418	1.00	24.66	PROT
ATOM	1723	CB	LEU	440	57.555	18.696	8.005	1.00	10.80	PROT
ATOM	1724	CG	LEU	440	56.501	19.658	8.541	1.00	8.60	PROT
ATOM	1725	CD1	LEU	440	57.152	20.985	8.855	1.00	17.69	PROT
ATOM	1726	CD2	LEU	440	55.410	19.847	7.522	1.00	15.71	PROT
ATOM	1727	C	LEU	440	58.245	16.578	6.912	1.00	29.61	PROT
ATOM	1728	O	LEU	440	58.506	16.526	5.718	1.00	32.37	PROT
ATOM	1729	N	HIS	441	58.971	15.954	7.830	1.00	28.12	PROT
ATOM	1730	CA	HIS	441	60.140	15.172	7.460	1.00	28.51	PROT
ATOM	1731	CB	HIS	441	60.783	14.564	8.705	1.00	36.77	PROT
ATOM	1732	C	HIS	441	59.724	14.081	6.497	1.00	31.94	PROT
ATOM	1733	O	HIS	441	60.461	13.725	5.579	1.00	49.29	PROT
ATOM	1734	N	MET	442	58.533	13.545	6.711	1.00	41.16	PROT
ATOM	1735	CA	MET	442	58.033	12.487	5.854	1.00	39.99	PROT
ATOM	1736	CB	MET	442	56.871	11.776	6.551	1.00	38.32	PROT
ATOM	1737	CG	MET	442	57.263	11.122	7.860	1.00	19.20	PROT
ATOM	1738	SD	MET	442	55.859	10.350	8.675	1.00	38.06	PROT
ATOM	1739	CE	MET	442	54.906	11.767	9.073	1.00	21.45	PROT
ATOM	1740	C	MET	442	57.599	13.031	4.495	1.00	35.68	PROT
ATOM	1741	O	MET	442	57.887	12.431	3.461	1.00	27.43	PROT
ATOM	1742	N	LYS	443	56.920	14.175	4.503	1.00	34.17	PROT
ATOM	1743	CA	LYS	443	56.447	14.796	3.268	1.00	34.33	PROT
ATOM	1744	CB	LYS	443	55.767	16.129	3.574	1.00	21.68	PROT
ATOM	1745	CG	LYS	443	54.303	15.989	3.953	1.00	26.95	PROT
ATOM	1746	CD	LYS	443	53.497	17.231	3.602	1.00	30.78	PROT
ATOM	1747	CE	LYS	443	52.204	16.848	2.861	1.00	56.06	PROT
ATOM	1748	NZ	LYS	443	50.931	17.261	3.564	1.00	45.26	PROT
ATOM	1749	C	LYS	443	57.570	15.007	2.251	1.00	37.81	PROT
ATOM	1750	O	LYS	443	57.325	15.049	1.041	1.00	38.26	PROT
ATOM	1751	N	VAL	444	58.798	15.130	2.741	1.00	25.12	PROT
ATOM	1752	CA	VAL	444	59.942	15.318	1.867	1.00	25.43	PROT
ATOM	1753	CB	VAL	444	60.802	16.531	2.334	1.00	29.15	PROT
ATOM	175									

ATOM	1758	N	GLU	445	60.127	12.888	1.903	1.00	39.84	PROT
ATOM	1759	CA	GLU	445	60.842	11.612	1.896	1.00	43.07	PROT
ATOM	1760	CB	GLU	445	61.429	11.360	3.282	1.00	50.55	PROT
ATOM	1761	CG	GLU	445	62.399	10.203	3.351	1.00	77.00	PROT
ATOM	1762	CD	GLU	445	63.569	10.495	4.267	1.00	98.21	PROT
ATOM	1763	OE1	GLU	445	64.251	9.538	4.701	1.00	100.00	PROT
ATOM	1764	OE2	GLU	445	63.804	11.690	4.554	1.00	100.00	PROT
ATOM	1765	C	GLU	445	59.989	10.408	1.491	1.00	43.41	PROT
ATOM	1766	O	GLU	445	60.466	9.274	1.511	1.00	48.80	PROT
ATOM	1767	N	CYS	446	58.731	10.644	1.137	1.00	38.17	PROT
ATOM	1768	CA	CYS	446	57.852	9.548	0.743	1.00	41.38	PROT
ATOM	1769	CB	CYS	446	57.066	9.035	1.965	1.00	40.61	PROT
ATOM	1770	SG	CYS	446	58.062	8.276	3.320	1.00	44.73	PROT
ATOM	1771	C	CYS	446	56.886	10.003	-0.362	1.00	45.83	PROT
ATOM	1772	O	CYS	446	56.466	11.184	-0.323	1.00	44.17	PROT
ATOM	1773	OT	CYS	446	56.570	9.180	-1.259	1.00	40.79	PROT
ATOM	1774	CB	GLU	449	52.635	12.140	-2.649	1.00	28.60	PROT
ATOM	1775	C	GLU	449	52.019	10.014	-1.526	1.00	38.06	PROT
ATOM	1776	O	GLU	449	50.873	10.220	-1.935	1.00	43.52	PROT
ATOM	1777	N	GLU	449	54.378	10.460	-2.167	1.00	17.78	PROT
ATOM	1778	CA	GLU	449	53.105	11.069	-1.689	1.00	33.80	PROT
ATOM	1779	N	LEU	450	52.387	8.880	-0.936	1.00	46.88	PROT
ATOM	1780	CA	LEU	450	51.432	7.808	-0.696	1.00	52.62	PROT
ATOM	1781	CB	LEU	450	52.101	6.436	-0.850	1.00	57.50	PROT
ATOM	1782	CG	LEU	450	53.338	6.066	-0.028	1.00	59.81	PROT
ATOM	1783	CD1	LEU	450	53.613	4.573	-0.198	1.00	51.33	PROT
ATOM	1784	CD2	LEU	450	54.544	6.890	-0.473	1.00	57.03	PROT
ATOM	1785	C	LEU	450	50.850	7.970	0.711	1.00	50.65	PROT
ATOM	1786	O	LEU	450	50.965	7.091	1.569	1.00	38.49	PROT
ATOM	1787	N	PHE	451	50.225	9.123	0.923	1.00	32.24	PROT
ATOM	1788	CA	PHE	451	49.602	9.478	2.188	1.00	32.64	PROT
ATOM	1789	CB	PHE	451	50.091	10.857	2.648	1.00	56.06	PROT
ATOM	1790	CG	PHE	451	51.534	10.895	3.056	1.00	61.73	PROT
ATOM	1791	CD1	PHE	451	52.523	10.366	2.235	1.00	66.92	PROT
ATOM	1792	CD2	PHE	451	51.905	11.486	4.256	1.00	58.76	PROT
ATOM	1793	CE1	PHE	451	53.860	10.430	2.604	1.00	69.17	PROT
ATOM	1794	CE2	PHE	451	53.231	11.556	4.635	1.00	61.48	PROT
ATOM	1795	CZ	PHE	451	54.214	11.028	3.809	1.00	71.95	PROT
ATOM	1796	C	PHE	451	48.081	9.548	2.025	1.00	30.67	PROT
ATOM	1797	O	PHE	451	47.571	10.429	1.324	1.00	38.49	PROT
ATOM	1798	N	PRO	452	47.336	8.627	2.672	1.00	19.14	PROT
ATOM	1799	CD	PRO	452	47.774	7.495	3.510	1.00	24.21	PROT
ATOM	1800	CA								



ATOM	1804	O	PRO	452	45.879	10.886	3.463	1.00	22.59	PROT
ATOM	1805	N	PRO	453	44.315	10.429	1.920	1.00	18.37	PROT
ATOM	1806	CD	PRO	453	43.653	9.540	0.951	1.00	3.83	PROT
ATOM	1807	CA	PRO	453	43.710	11.766	1.960	1.00	14.00	PROT
ATOM	1808	CB	PRO	453	42.502	11.649	1.032	1.00	20.04	PROT
ATOM	1809	CG	PRO	453	42.316	10.163	0.807	1.00	19.43	PROT
ATOM	1810	C	PRO	453	43.321	12.277	3.346	1.00	14.70	PROT
ATOM	1811	O	PRO	453	43.609	13.422	3.682	1.00	9.70	PROT
ATOM	1812	N	LEU	454	42.667	11.446	4.152	1.00	25.39	PROT
ATOM	1813	CA	LEU	454	42.261	11.886	5.491	1.00	28.61	PROT
ATOM	1814	CB	LEU	454	41.463	10.804	6.217	1.00	17.29	PROT
ATOM	1815	CG	LEU	454	40.893	11.224	7.572	1.00	9.05	PROT
ATOM	1816	CD1	LEU	454	40.174	12.547	7.435	1.00	17.23	PROT
ATOM	1817	CD2	LEU	454	39.946	10.148	8.079	1.00	8.05	PROT
ATOM	1818	C	LEU	454	43.479	12.234	6.316	1.00	23.36	PROT
ATOM	1819	O	LEU	454	43.484	13.225	7.037	1.00	10.99	PROT
ATOM	1820	N	PHE	455	44.503	11.394	6.205	1.00	14.26	PROT
ATOM	1821	CA	PHE	455	45.769	11.595	6.902	1.00	15.33	PROT
ATOM	1822	CB	PHE	455	46.761	10.496	6.501	1.00	26.32	PROT
ATOM	1823	CG	PHE	455	48.138	10.644	7.108	1.00	43.03	PROT
ATOM	1824	CD1	PHE	455	48.305	11.094	8.414	1.00	43.52	PROT
ATOM	1825	CD2	PHE	455	49.270	10.282	6.380	1.00	41.44	PROT
ATOM	1826	CE1	PHE	455	49.576	11.176	8.987	1.00	37.77	PROT
ATOM	1827	CE2	PHE	455	50.536	10.363	6.947	1.00	49.43	PROT
ATOM	1828	CZ	PHE	455	50.686	10.811	8.255	1.00	39.99	PROT
ATOM	1829	C	PHE	455	46.313	12.956	6.500	1.00	19.37	PROT
ATOM	1830	O	PHE	455	46.945	13.646	7.298	1.00	29.31	PROT
ATOM	1831	N	LEU	456	46.048	13.345	5.257	1.00	17.16	PROT
ATOM	1832	CA	LEU	456	46.527	14.625	4.750	1.00	20.15	PROT
ATOM	1833	CB	LEU	456	46.572	14.603	3.218	1.00	35.14	PROT
ATOM	1834	CG	LEU	456	47.593	13.660	2.568	1.00	40.45	PROT
ATOM	1835	CD1	LEU	456	47.233	13.456	1.116	1.00	44.38	PROT
ATOM	1836	CD2	LEU	456	48.990	14.234	2.680	1.00	34.88	PROT
ATOM	1837	C	LEU	456	45.680	15.800	5.226	1.00	20.37	PROT
ATOM	1838	O	LEU	456	46.207	16.866	5.548	1.00	29.61	PROT
ATOM	1839	N	GLU	457	44.367	15.607	5.280	1.00	13.06	PROT
ATOM	1840	CA	GLU	457	43.483	16.675	5.713	1.00	14.14	PROT
ATOM	1841	CB	GLU	457	42.037	16.256	5.516	1.00	29.57	PROT
ATOM	1842	C	GLU	457	43.731	17.058	7.173	1.00	14.95	PROT
ATOM	1843	O	GLU	457	43.771	18.237	7.514	1.00	15.98	PROT
ATOM	1844	N	VAL	458	43.901	16.051	8.026	1.00	26.34	PROT
ATOM	1845	CA	VAL	458	44.143	16.260	9.455	1.00	24.39	PROT
ATOM	184									



ATOM	1850	O	VAL	458	45.364	18.062	10.439	1.00	18.85	PROT
ATOM	1851	N	PHE	459	46.557	16.546	9.308	1.00	16.05	PROT
ATOM	1852	CA	PHE	459	47.840	17.174	9.586	1.00	20.28	PROT
ATOM	1853	CB	PHE	459	48.862	16.072	9.846	1.00	20.26	PROT
ATOM	1854	CG	PHE	459	48.389	15.055	10.833	1.00	27.22	PROT
ATOM	1855	CD1	PHE	459	47.917	13.822	10.408	1.00	28.01	PROT
ATOM	1856	CD2	PHE	459	48.390	15.339	12.204	1.00	40.66	PROT
ATOM	1857	CE1	PHE	459	47.447	12.876	11.334	1.00	21.78	PROT
ATOM	1858	CE2	PHE	459	47.922	14.402	13.140	1.00	25.98	PROT
ATOM	1859	CZ	PHE	459	47.450	13.172	12.702	1.00	17.63	PROT
ATOM	1860	C	PHE	459	48.381	18.152	8.540	1.00	23.03	PROT
ATOM	1861	O	PHE	459	49.601	18.311	8.416	1.00	27.34	PROT
ATOM	1862	N	GLU	460	47.480	18.816	7.815	1.00	33.88	PROT
ATOM	1863	CA	GLU	460	47.846	19.774	6.767	1.00	36.60	PROT
ATOM	1864	CB	GLU	460	48.930	20.732	7.257	1.00	46.04	PROT
ATOM	1865	CG	GLU	460	48.406	21.899	8.054	1.00	67.27	PROT
ATOM	1866	CD	GLU	460	47.298	22.636	7.339	1.00	71.34	PROT
ATOM	1867	OE1	GLU	460	47.448	23.859	7.121	1.00	71.99	PROT
ATOM	1868	OE2	GLU	460	46.280	21.993	6.998	1.00	72.73	PROT
ATOM	1869	C	GLU	460	48.353	19.037	5.535	1.00	46.31	PROT
ATOM	1870	O	GLU	460	48.642	17.829	5.655	1.00	51.79	PROT
ATOM	1871	OT	GLU	460	48.461	19.669	4.462	1.00	60.92	PROT
ATOM	1872	C1	GC1	1	47.011	4.539	15.912	1.00	29.38	LIGA
ATOM	1873	C2	GC1	1	51.292	6.537	13.571	1.00	17.11	LIGA
ATOM	1874	C3	GC1	1	47.393	4.205	14.573	1.00	33.72	LIGA
ATOM	1875	C4	GC1	1	52.119	6.409	12.400	1.00	19.76	LIGA
ATOM	1876	C5	GC1	1	48.689	4.481	14.089	1.00	25.02	LIGA
ATOM	1877	C6	GC1	1	52.344	7.525	11.539	1.00	17.51	LIGA
ATOM	1878	C7	GC1	1	49.684	5.122	14.949	1.00	23.99	LIGA
ATOM	1879	C8	GC1	1	51.722	8.778	11.873	1.00	20.21	LIGA
ATOM	1880	C9	GC1	1	49.283	5.452	16.318	1.00	18.19	LIGA
ATOM	1881	C10	GC1	1	50.906	8.928	13.018	1.00	15.43	LIGA
ATOM	1882	C11	GC1	1	47.973	5.163	16.779	1.00	30.64	LIGA
ATOM	1883	C12	GC1	1	50.696	7.827	13.850	1.00	25.06	LIGA
ATOM	1884	O5	GC1	1	45.700	4.254	16.325	1.00	28.60	LIGA
ATOM	1885	C14	GC1	1	53.198	7.459	10.291	1.00	20.30	LIGA
ATOM	1886	C15	GC1	1	45.305	3.866	17.666	1.00	18.51	LIGA
ATOM	1887	C16	GC1	1	52.423	6.824	9.131	1.00	17.21	LIGA
ATOM	1888	C17	GC1	1	43.816	4.078	17.872	1.00	21.43	LIGA
ATOM	1889	C18	GC1	1	54.514	6.689	10.543	1.00	24.97	LIGA
ATOM	1890	C19	GC1	1	48.994	4.093	12.664	1.00	33.46	LIGA
ATOM	1891	C20	GC1	1	50.243	6.110	17.278	1.00	27.69	LIGA
ATOM	1892	O1	GC1	1						



## APPENDIX 8

### TRBGC1.PDB

REMARK TR-beta GC-2 Full length numbering  
 REMARK refinement resolution: 100.00 - 2.40 A starting r= 0.2602 free\_r= 0.2960  
 REMARK - final r= 0.2532 free\_r= 0.2894  
 REMARK sg= P3(1)21 a= 68.9 b= 68.9 c= 131.5 alpha= 90 beta= 90 gamma= 120  
 REMARK theoretical total number of refl. in resol. range: 14710 ( 100.0 % )  
 REMARK number of unobserved reflections (no entry or |F|=0): 336 ( 2.3 % )  
 REMARK number of reflections rejected: 0 ( 0.0 % )  
 REMARK total number of reflections used: 14374 ( 97.7 % )  
 REMARK number of reflections in working set: 13656 ( 92.8 % )  
 REMARK number of reflections in test set: 718 ( 4.9 % )  
 REMARK  
 REMARK ALA 199 to ALA 201 from His-tag  
 REMARK  
 REMARK Four cacodylate-modified cysteines (CYA)  
 REMARK Cys294, Cys298, Cys388, Cys434  
 REMARK cacodylate modeled as single arsenic atom  
 REMARK  
 REMARK side chain of certain residues modeled as ALA due to poor density;  
 REMARK however, residue name reflects true residue for clarity  
 REMARK  
 REMARK amino acid sequence confirmed,  
 REMARK differing from that reported by Weinberger et. al.  
 REMARK in the following codons:  
 REMARK 243 Pro - Arg  
 REMARK 337 Ile - Thr  
 REMARK 451 Leu - Phe  
 REMARK as reported by Sakurai et. al.  
 REMARK note also correction of initiation codon,  
 REMARK yielding a polypeptide of 461 amino acids

JRNL AUTH A.SAKURAI,A.NAKAI,L.J.DEGROOT  
 JRNL TITL STRUCTURAL ANALYSIS OF HUMAN THYROID HORMONE RECEPTOR  
 JRNL TITL2 BETA GENE  
 JRNL REF MOL.CELL.ENDO. V.71 1990  
 JRNL AUTH C.WEINBERGER, C.C.THOMPSON,R.LEBO,D.J.GRUOL,R.M.EVANS  
 JRNL TITL THE C-ERB-A GENE ENCODES A THYROID HORMONE RECEPTOR  
 JRNL REF NATURE V.324 6098 1986

ATOM	1	CB	ALA	199	36.564	26.104	43.169	1.00	73.87
ATOM	2	C	ALA	199	34.723	26.996	44.613	1.00	78.22
ATOM	3	O	ALA	199	34.741	28.230	44.568	1.00	81.84
ATOM	4	N	ALA	199	34.389	26.744	42.166	1.00	77.76
ATOM	5	CA	ALA	199	35.048	26.165	43.375	1.00	77.98

ATOM	6	N	ALA	200	34.428	26.309	45.713	1.00	77.78
ATOM	7	CA	ALA	200	34.098	26.961	46.984	1.00	77.03
ATOM	8	CB	ALA	200	32.761	27.693	46.865	1.00	79.04
ATOM	9	C	ALA	200	34.028	25.897	48.084	1.00	75.79
ATOM	10	O	ALA	200	34.877	25.857	48.978	1.00	71.58
ATOM	11	N	ALA	201	33.005	25.050	48.010	1.00	73.70
ATOM	12	CA	ALA	201	32.838	23.968	48.972	1.00	70.15
ATOM	13	CB	ALA	201	31.468	23.328	48.809	1.00	71.16
ATOM	14	C	ALA	201	33.934	22.963	48.642	1.00	67.54
ATOM	15	O	ALA	201	34.218	22.044	49.413	1.00	67.14
ATOM	16	N	GLU	202	34.540	23.164	47.476	1.00	62.05
ATOM	17	CA	GLU	202	35.624	22.325	46.975	1.00	59.45
ATOM	18	CB	GLU	202	35.835	22.621	45.482	1.00	55.12
ATOM	19	CG	GLU	202	36.820	21.716	44.749	1.00	56.25
ATOM	20	CD	GLU	202	36.382	20.260	44.723	1.00	54.99
ATOM	21	OE1	GLU	202	35.216	19.990	44.361	1.00	53.83
ATOM	22	OE2	GLU	202	37.210	19.385	45.050	1.00	59.90
ATOM	23	C	GLU	202	36.885	22.674	47.770	1.00	55.96
ATOM	24	O	GLU	202	37.472	21.823	48.435	1.00	52.90
ATOM	25	N	GLU	203	37.282	23.943	47.698	1.00	54.95
ATOM	26	CA	GLU	203	38.464	24.434	48.390	1.00	55.59
ATOM	27	CB	GLU	203	38.632	25.924	48.126	1.00	53.21
ATOM	28	C	GLU	203	38.415	24.171	49.894	1.00	56.30
ATOM	29	O	GLU	203	39.445	23.948	50.526	1.00	58.70
ATOM	30	N	LEU	204	37.213	24.193	50.462	1.00	57.14
ATOM	31	CA	LEU	204	37.038	23.966	51.893	1.00	56.93
ATOM	32	CB	LEU	204	35.658	24.465	52.338	1.00	58.31
ATOM	33	CG	LEU	204	35.348	24.508	53.839	1.00	51.69
ATOM	34	CD1	LEU	204	36.314	25.446	54.549	1.00	44.38
ATOM	35	CD2	LEU	204	33.920	24.986	54.039	1.00	52.44
ATOM	36	C	LEU	204	37.198	22.489	52.246	1.00	58.20
ATOM	37	O	LEU	204	37.831	22.155	53.252	1.00	58.99
ATOM	38	N	GLN	205	36.620	21.607	51.431	1.00	58.26
ATOM	39	CA	GLN	205	36.736	20.167	51.657	1.00	55.38
ATOM	40	CB	GLN	205	35.993	19.377	50.584	1.00	54.52
ATOM	41	CG	GLN	205	34.498	19.324	50.741	1.00	53.33
ATOM	42	CD	GLN	205	33.854	18.520	49.629	1.00	53.40
ATOM	43	OE1	GLN	205	33.850	18.939	48.473	1.00	51.68
ATOM	44	NE2	GLN	205	33.325	17.352	49.968	1.00	51.34
ATOM	45	C	GLN	205	38.200	19.775	51.608	1.00	55.05
ATOM	46	O	GLN	205	38.665	18.964	52.407	1.00	53.63
ATOM	47	N	LYS	206	38.918	20.348	50.648	1.00	53.55
ATOM	48	CA	LYS	206	40.337	20.078	50.493	1.00	57.40
ATOM	49	CB	LYS	206	40.896	20.814	49.269	1.00	58.94
ATOM	50	CG	LYS	206	40.300	20.375	47.941	1.00	67.73
ATOM	51	CD	LYS	206	40.921	21.141	46.781		

ATOM	52	CE	LYS	206	40.346	20.695	45.445	1.00	75.60
ATOM	53	NZ	LYS	206	40.945	21.445	44.304	1.00	77.08
ATOM	54	C	LYS	206	41.053	20.559	51.747	1.00	53.98
ATOM	55	O	LYS	206	41.905	19.866	52.300	1.00	53.49
ATOM	56	N	SER	207	40.680	21.757	52.184	1.00	53.61
ATOM	57	CA	SER	207	41.254	22.386	53.364	1.00	51.49
ATOM	58	CB	SER	207	40.546	23.715	53.619	1.00	51.01
ATOM	59	OG	SER	207	41.108	24.383	54.731	1.00	63.00
ATOM	60	C	SER	207	41.178	21.502	54.616	1.00	49.49
ATOM	61	O	SER	207	42.073	21.538	55.465	1.00	47.44
ATOM	62	N	ILE	208	40.117	20.707	54.725	1.00	44.39
ATOM	63	CA	ILE	208	39.938	19.829	55.874	1.00	45.99
ATOM	64	CB	ILE	208	38.421	19.627	56.174	1.00	44.50
ATOM	65	CG2	ILE	208	38.226	18.801	57.445	1.00	49.37
ATOM	66	CG1	ILE	208	37.766	20.993	56.385	1.00	42.73
ATOM	67	CD1	ILE	208	36.266	20.941	56.567	1.00	44.13
ATOM	68	C	ILE	208	40.614	18.477	55.643	1.00	47.80
ATOM	69	O	ILE	208	40.735	17.666	56.562	1.00	49.81
ATOM	70	N	GLY	209	41.059	18.238	54.412	1.00	51.31
ATOM	71	CA	GLY	209	41.728	16.983	54.107	1.00	46.85
ATOM	72	C	GLY	209	40.813	15.896	53.573	1.00	48.31
ATOM	73	O	GLY	209	41.203	14.730	53.485	1.00	47.75
ATOM	74	N	HIS	210	39.582	16.274	53.237	1.00	46.79
ATOM	75	CA	HIS	210	38.622	15.326	52.686	1.00	47.34
ATOM	76	CB	HIS	210	37.200	15.739	53.068	1.00	49.39
ATOM	77	C	HIS	210	38.796	15.350	51.162	1.00	45.47
ATOM	78	O	HIS	210	38.924	16.420	50.566	1.00	41.32
ATOM	79	N	LYS	211	38.829	14.176	50.545	1.00	45.76
ATOM	80	CA	LYS	211	38.991	14.095	49.090	1.00	43.42
ATOM	81	CB	LYS	211	39.892	12.910	48.715	1.00	46.72
ATOM	82	CG	LYS	211	41.210	12.815	49.497	1.00	56.48
ATOM	83	CD	LYS	211	42.068	14.089	49.486	1.00	60.93
ATOM	84	CE	LYS	211	42.562	14.496	48.103	1.00	61.95
ATOM	85	NZ	LYS	211	41.485	15.024	47.218	1.00	69.93
ATOM	86	C	LYS	211	37.609	13.917	48.473	1.00	35.68
ATOM	87	O	LYS	211	37.019	12.847	48.557	1.00	33.58
ATOM	88	N	PRO	212	37.077	14.972	47.828	1.00	35.64
ATOM	89	CD	PRO	212	37.654	16.304	47.584	1.00	38.60
ATOM	90	CA	PRO	212	35.748	14.896	47.211	1.00	38.35
ATOM	91	CB	PRO	212	35.537	16.318	46.682	1.00	38.95
ATOM	92	CG	PRO	212	36.409	17.156	47.604	1.00	42.00
ATOM	93	C	PRO	212	35.635	13.865	46.096	1.00	38.78
ATOM	94	O	PRO	212	36.546	13.714	45.280	1.00	34.64
ATOM	95	N	GLU	213	34.517	13.153	46.077	1.00	40.31
ATOM	96	CA	GLU	213	34.256	12.160	45.049	1.00	43.87
ATOM	97	CB	GLU	213	33.722	10.873	45.684	1.00	45.16



ATOM	98	CG	GLU	213	34.616	10.344	46.800	1.00	47.60
ATOM	99	CD	GLU	213	34.404	8.870	47.088	1.00	50.68
ATOM	100	OE1	GLU	213	33.240	8.416	47.072	1.00	59.18
ATOM	101	OE2	GLU	213	35.402	8.167	47.353	1.00	49.06
ATOM	102	C	GLU	213	33.234	12.796	44.083	1.00	45.96
ATOM	103	O.	GLU	213	32.703	13.876	44.368	1.00	43.13
ATOM	104	N	PRO	214	32.953	12.154	42.933	1.00	46.52
ATOM	105	CD	PRO	214	33.459	10.884	42.391	1.00	46.44
ATOM	106	CA	PRO	214	31.995	12.737	41.982	1.00	47.52
ATOM	107	CB	PRO	214	32.040	11.750	40.813	1.00	45.40
ATOM	108	CG	PRO	214	33.445	11.181	40.913	1.00	49.89
ATOM	109	C	PRO	214	30.564	12.969	42.465	1.00	45.70
ATOM	110	O	PRO	214	29.972	12.112	43.121	1.00	44.49
ATOM	111	N	THR	215	30.013	14.136	42.129	1.00	45.24
ATOM	112	CA	THR	215	28.629	14.447	42.483	1.00	49.36
ATOM	113	CB	THR	215	28.312	15.949	42.330	1.00	44.86
ATOM	114	OG1	THR	215	28.253	16.285	40.942	1.00	52.26
ATOM	115	CG2	THR	215	29.387	16.793	42.992	1.00	39.43
ATOM	116	C	THR	215	27.791	13.673	41.464	1.00	52.51
ATOM	117	O	THR	215	28.326	13.192	40.465	1.00	53.48
ATOM	118	N	ASP	216	26.491	13.543	41.712	1.00	58.81
ATOM	119	CA	ASP	216	25.603	12.810	40.805	1.00	61.51
ATOM	120	CB	ASP	216	24.150	12.941	41.270	1.00	70.57
ATOM	121	CG	ASP	216	23.902	12.257	42.595	1.00	78.07
ATOM	122	OD1	ASP	216	24.042	11.018	42.660	1.00	82.31
ATOM	123	OD2	ASP	216	23.572	12.962	43.571	1.00	86.55
ATOM	124	C	ASP	216	25.706	13.277	39.356	1.00	58.42
ATOM	125	O	ASP	216	25.695	12.464	38.429	1.00	56.85
ATOM	126	N	GLU	217	25.798	14.587	39.167	1.00	54.92
ATOM	127	CA	GLU	217	25.905	15.156	37.833	1.00	53.37
ATOM	128	CB	GLU	217	25.861	16.682	37.906	1.00	51.02
ATOM	129	C	GLU	217	27.211	14.692	37.195	1.00	53.55
ATOM	130	O	GLU	217	27.239	14.301	36.027	1.00	54.33
ATOM	131	N	GLU	218	28.290	14.726	37.975	1.00	49.20
ATOM	132	CA	GLU	218	29.593	14.310	37.486	1.00	45.94
ATOM	133	CB	GLU	218	30.674	14.601	38.530	1.00	43.43
ATOM	134	CG	GLU	218	30.787	16.069	38.878	1.00	40.86
ATOM	135	CD	GLU	218	31.930	16.347	39.826	1.00	39.88
ATOM	136	OE1	GLU	218	32.000	15.667	40.875	1.00	37.61
ATOM	137	OE2	GLU	218	32.748	17.250	39.529	1.00	34.01
ATOM	138	C	GLU	218	29.624	12.838	37.101	1.00	44.71
ATOM	139	O	GLU	218	30.275	12.471	36.130	1.00	45.31
ATOM	140	N	TRP	219	28.935	11.991	37.863	1.00	44.02
ATOM	141	CA	TRP	219	28.892	10.572	37.539	1.00	46.97
ATOM	142	CB	TRP	219	28.183	9.762	38.630	1.00	48.42
ATOM	143	CG	TRP	219					

ATOM	144	CD2 TRP	219	30.167	8.572	39.879	1.00	55.24
ATOM	145	CE2 TRP	219	30.659	8.610	41.201	1.00	53.67
ATOM	146	CE3 TRP	219	30.795	7.745	38.938	1.00	54.55
ATOM	147	CD1 TRP	219	28.902	10.000	41.074	1.00	55.75
ATOM	148	NE1 TRP	219	29.868	9.491	41.912	1.00	54.43
ATOM	149	CZ2 TRP	219	31.771	7.846	41.622	1.00	52.54
ATOM	150	CZ3 TRP	219	31.912	6.975	39.353	1.00	55.17
ATOM	151	CH2 TRP	219	32.380	7.038	40.690	1.00	55.59
ATOM	152	C TRP	219	28.167	10.356	36.216	1.00	47.32
ATOM	153	O TRP	219	28.433	9.384	35.503	1.00	43.56
ATOM	154	N GLU	220	27.247	11.259	35.898	1.00	49.91
ATOM	155	CA GLU	220	26.497	11.155	34.655	1.00	53.57
ATOM	156	CB GLU	220	25.274	12.075	34.694	1.00	58.18
ATOM	157	CG GLU	220	24.323	11.876	33.526	1.00	73.13
ATOM	158	CD GLU	220	23.082	12.742	33.630	1.00	80.06
ATOM	159	OE1 GLU	220	22.348	12.619	34.636	1.00	82.12
ATOM	160	OE2 GLU	220	22.839	13.545	32.701	1.00	82.78
ATOM	161	C GLU	220	27.419	11.534	33.497	1.00	50.51
ATOM	162	O GLU	220	27.399	10.899	32.443	1.00	49.94
ATOM	163	N LEU	221	28.232	12.567	33.711	1.00	43.71
ATOM	164	CA LEU	221	29.187	13.019	32.702	1.00	42.81
ATOM	165	CB LEU	221	29.868	14.317	33.155	1.00	39.21
ATOM	166	CG LEU	221	30.945	14.949	32.261	1.00	36.34
ATOM	167	CD1 LEU	221	30.339	15.351	30.922	1.00	36.93
ATOM	168	CD2 LEU	221	31.535	16.164	32.949	1.00	24.18
ATOM	169	C LEU	221	30.234	11.928	32.505	1.00	43.46
ATOM	170	O LEU	221	30.618	11.621	31.375	1.00	45.25
ATOM	171	N ILE	222	30.683	11.342	33.614	1.00	39.09
ATOM	172	CA ILE	222	31.677	10.273	33.586	1.00	35.47
ATOM	173	CB ILE	222	32.031	9.811	35.037	1.00	33.74
ATOM	174	CG2 ILE	222	32.822	8.505	35.018	1.00	28.86
ATOM	175	CG1 ILE	222	32.813	10.918	35.745	1.00	33.33
ATOM	176	CD1 ILE	222	33.111	10.646	37.199	1.00	34.85
ATOM	177	C ILE	222	31.139	9.098	32.781	1.00	34.26
ATOM	178	O ILE	222	31.877	8.427	32.070	1.00	31.90
ATOM	179	N LYS	223	29.840	8.860	32.908	1.00	39.49
ATOM	180	CA LYS	223	29.168	7.775	32.210	1.00	44.43
ATOM	181	CB LYS	223	27.696	7.733	32.635	1.00	50.81
ATOM	182	CG LYS	223	26.845	6.693	31.929	1.00	62.51
ATOM	183	CD LYS	223	25.379	6.856	32.313	1.00	72.22
ATOM	184	CE LYS	223	24.487	5.855	31.591	1.00	74.55
ATOM	185	NZ LYS	223	23.045	6.057	31.925	1.00	75.78
ATOM	186	C LYS	223	29.266	7.983	30.691	1.00	42.81
ATOM	187	O LYS	223	29.640	7.078	29.946	1.00	40.36
ATOM	188	N THR	224	28.924	9.194	30.257	1.00	39.89
ATOM	189	CA THR	224	28.948	9.566	28.850	1.00	39.93



ATOM	236	N	ALA	231	33.236	2.698	23.230	1.00	45.59
ATOM	237	CA	ALA	231	32.580	2.403	21.961	1.00	47.84
ATOM	238	CB	ALA	231	31.297	3.227	21.832	1.00	45.08
ATOM	239	C	ALA	231	33.487	2.666	20.761	1.00	48.04
ATOM	240	O	ALA	231	33.364	2.012	19.727	1.00	49.95
ATOM	241	N-	THR	232	34.403	3.619	20.907	1.00	47.26
ATOM	242	CA	THR	232	35.312	3.973	19.824	1.00	43.64
ATOM	243	CB	THR	232	35.379	5.502	19.629	1.00	41.93
ATOM	244	OG1	THR	232	35.945	6.117	20.797	1.00	39.10
ATOM	245	CG2	THR	232	33.985	6.065	19.382	1.00	29.80
ATOM	246	C	THR	232	36.720	3.458	20.046	1.00	43.97
ATOM	247	O	THR	232	37.629	3.791	19.292	1.00	40.55
ATOM	248	N	ASN	233	36.905	2.648	21.081	1.00	48.62
ATOM	249	CA	ASN	233	38.218	2.101	21.368	1.00	58.62
ATOM	250	CB	ASN	233	38.473	2.092	22.876	1.00	62.44
ATOM	251	CG	ASN	233	39.909	1.765	23.223	1.00	68.35
ATOM	252	OD1	ASN	233	40.843	2.401	22.724	1.00	65.50
ATOM	253	ND2	ASN	233	40.098	0.776	24.090	1.00	74.29
ATOM	254	C	ASN	233	38.282	0.690	20.802	1.00	65.06
ATOM	255	O	ASN	233	37.748	-0.257	21.382	1.00	69.47
ATOM	256	N	ALA	234	38.934	0.577	19.645	1.00	68.80
ATOM	257	CA	ALA	234	39.098	-0.672	18.909	1.00	70.98
ATOM	258	CB	ALA	234	40.215	-0.508	17.886	1.00	71.43
ATOM	259	C	ALA	234	39.353	-1.919	19.753	1.00	73.83
ATOM	260	O	ALA	234	40.193	-1.911	20.652	1.00	74.33
ATOM	261	N	GLN	235	38.615	-2.983	19.434	1.00	75.07
ATOM	262	CA	GLN	235	38.720	-4.281	20.103	1.00	76.32
ATOM	263	CB	GLN	235	40.130	-4.856	19.912	1.00	76.98
ATOM	264	CG	GLN	235	40.429	-5.417	18.516	1.00	77.07
ATOM	265	CD	GLN	235	40.142	-4.444	17.377	1.00	80.85
ATOM	266	OE1	GLN	235	38.985	-4.144	17.072	1.00	82.01
ATOM	267	NE2	GLN	235	41.201	-3.949	16.742	1.00	78.80
ATOM	268	C	GLN	235	38.351	-4.293	21.586	1.00	77.15
ATOM	269	O	GLN	235	38.217	-5.361	22.190	1.00	76.06
ATOM	270	N	GLY	236	38.188	-3.103	22.161	1.00	77.46
ATOM	271	CA	GLY	236	37.818	-2.974	23.562	1.00	78.37
ATOM	272	C	GLY	236	38.620	-3.783	24.566	1.00	79.43
ATOM	273	O	GLY	236	39.826	-3.575	24.736	1.00	79.47
ATOM	274	N	SER	237	37.937	-4.711	25.234	1.00	77.98
ATOM	275	CA	SER	237	38.544	-5.561	26.253	1.00	76.49
ATOM	276	CB	SER	237	37.475	-6.462	26.874	1.00	76.46
ATOM	277	C	SER	237	39.712	-6.412	25.765	1.00	75.35
ATOM	278	O	SER	237	40.858	-6.181	26.152	1.00	75.47
ATOM	279	N	HIS	238	39.421	-7.397	24.922	1.00	75.56
ATOM	280	CA	HIS	238	40.451	-8.294	24.409	1.00	75.46
ATOM	281	CB	HIS	238	39.837	-9.654	24.076	1.00	75.85



ATOM	282	C	HIS	238	41.185	-7.751	23.191	1.00	74.10
ATOM	283	O	HIS	238	40.610	-7.638	22.109	1.00	75.34
ATOM	284	N	TRP	239	42.459	-7.417	23.381	1.00	73.39
ATOM	285	CA	TRP	239	43.300	-6.907	22.302	1.00	74.02
ATOM	286	CB	TRP	239	43.556	-5.402	22.460	1.00	81.77
ATOM	287	CG	TRP	239	44.190	-5.023	23.761	1.00	89.67
ATOM	288	CD2	TRP	239	45.597	-4.797	24.008	1.00	93.19
ATOM	289	CE2	TRP	239	45.744	-4.527	25.384	1.00	95.46
ATOM	290	CE3	TRP	239	46.732	-4.793	23.186	1.00	95.35
ATOM	291	CD1	TRP	239	43.566	-4.888	24.972	1.00	94.16
ATOM	292	NE1	TRP	239	44.483	-4.591	25.954	1.00	97.48
ATOM	293	CZ2	TRP	239	46.993	-4.262	25.981	1.00	96.23
ATOM	294	CZ3	TRP	239	47.992	-4.528	23.778	1.00	96.75
ATOM	295	CH2	TRP	239	48.101	-4.262	25.164	1.00	97.32
ATOM	296	C	TRP	239	44.633	-7.649	22.283	1.00	70.77
ATOM	297	O	TRP	239	45.339	-7.644	21.274	1.00	71.70
ATOM	298	N	LYS	240	44.978	-8.276	23.405	1.00	67.10
ATOM	299	CA	LYS	240	46.219	-9.040	23.519	1.00	65.63
ATOM	300	CB	LYS	240	46.387	-9.569	24.946	1.00	66.65
ATOM	301	CG	LYS	240	46.379	-8.504	26.030	1.00	69.83
ATOM	302	CD	LYS	240	47.664	-7.691	26.069	1.00	71.49
ATOM	303	CE	LYS	240	48.839	-8.515	26.573	1.00	71.31
ATOM	304	NZ	LYS	240	50.071	-7.684	26.691	1.00	72.23
ATOM	305	C	LYS	240	46.143	-10.222	22.555	1.00	66.19
ATOM	306	O	LYS	240	47.075	-10.493	21.797	1.00	65.20
ATOM	307	N	ASN	241	45.010	-10.923	22.598	1.00	66.69
ATOM	308	CA	ASN	241	44.773	-12.089	21.750	1.00	67.53
ATOM	309	CB	ASN	241	43.503	-12.813	22.213	1.00	67.98
ATOM	310	CG	ASN	241	43.504	-13.096	23.704	1.00	70.19
ATOM	311	OD1	ASN	241	44.410	-13.744	24.227	1.00	71.37
ATOM	312	ND2	ASN	241	42.483	-12.605	24.400	1.00	71.48
ATOM	313	C	ASN	241	44.621	-11.681	20.286	1.00	66.62
ATOM	314	O	ASN	241	44.882	-12.475	19.382	1.00	64.76
ATOM	315	N	LYS	242	44.196	-10.436	20.070	1.00	66.86
ATOM	316	CA	LYS	242	43.989	-9.882	18.732	1.00	67.46
ATOM	317	CB	LYS	242	42.982	-8.731	18.799	1.00	67.93
ATOM	318	CG	LYS	242	41.601	-9.138	19.279	1.00	71.52
ATOM	319	CD	LYS	242	40.876	-9.986	18.246	1.00	74.32
ATOM	320	CE	LYS	242	40.449	-9.160	17.043	1.00	74.41
ATOM	321	NZ	LYS	242	39.455	-8.120	17.436	1.00	74.44
ATOM	322	C	LYS	242	45.281	-9.367	18.097	1.00	66.28
ATOM	323	O	LYS	242	45.414	-9.334	16.874	1.00	67.61
ATOM	324	N	ARG	243	46.225	-8.961	18.938	1.00	64.19
ATOM	325	CA	ARG	243	47.497	-8.422	18.478	1.00	62.43
ATOM	326	CB	ARG	243	48.376	-8.070	19.685	1.00	60.12
ATOM	327	C	ARG	243	48.261	-9.3			



ATOM	328	O	ARG	243	48.585	-10.484	17.891	1.00	63.96
ATOM	329	N	LYS	244	48.531	-8.853	16.334	1.00	62.41
ATOM	330	CA	LYS	244	49.303	-9.593	15.339	1.00	61.57
ATOM	331	CB	LYS	244	48.601	-9.607	13.972	1.00	63.68
ATOM	332	CG	LYS	244	47.210	-10.231	13.970	1.00	71.29
ATOM	333	CD	LYS	244	46.666	-10.441	12.549	1.00	73.83
ATOM	334	CE	LYS	244	46.505	-9.139	11.767	1.00	74.71
ATOM	335	NZ	LYS	244	45.542	-8.199	12.407	1.00	73.32
ATOM	336	C	LYS	244	50.613	-8.824	15.223	1.00	59.30
ATOM	337	O	LYS	244	50.637	-7.716	14.686	1.00	56.34
ATOM	338	N	PHE	245	51.690	-9.405	15.744	1.00	57.06
ATOM	339	CA	PHE	245	52.996	-8.757	15.704	1.00	59.01
ATOM	340	CB	PHE	245	54.034	-9.588	16.467	1.00	59.62
ATOM	341	CG	PHE	245	53.704	-9.783	17.934	1.00	66.60
ATOM	342	CD1	PHE	245	52.656	-10.626	18.329	1.00	67.17
ATOM	343	CD2	PHE	245	54.427	-9.096	18.918	1.00	69.25
ATOM	344	CE1	PHE	245	52.320	-10.789	19.699	1.00	69.92
ATOM	345	CE2	PHE	245	54.111	-9.240	20.294	1.00	70.50
ATOM	346	CZ	PHE	245	53.051	-10.091	20.686	1.00	70.89
ATOM	347	C	PHE	245	53.463	-8.537	14.272	1.00	60.68
ATOM	348	O	PHE	245	53.433	-9.455	13.447	1.00	62.37
ATOM	349	N	LEU	246	53.880	-7.311	13.976	1.00	60.10
ATOM	350	CA	LEU	246	54.359	-6.968	12.642	1.00	59.44
ATOM	351	CB	LEU	246	54.654	-5.464	12.560	1.00	57.43
ATOM	352	CG	LEU	246	54.937	-4.851	11.183	1.00	54.41
ATOM	353	CD1	LEU	246	53.681	-4.931	10.320	1.00	52.43
ATOM	354	CD2	LEU	246	55.358	-3.398	11.343	1.00	51.69
ATOM	355	C	LEU	246	55.638	-7.772	12.425	1.00	62.05
ATOM	356	O	LEU	246	56.447	-7.923	13.346	1.00	59.85
ATOM	357	N	PRO	247	55.836	-8.312	11.203	1.00	63.33
ATOM	358	CD	PRO	247	54.990	-8.230	10.001	1.00	64.44
ATOM	359	CA	PRO	247	57.036	-9.102	10.910	1.00	63.56
ATOM	360	CB	PRO	247	56.917	-9.327	9.404	1.00	64.42
ATOM	361	CG	PRO	247	55.413	-9.481	9.251	1.00	64.90
ATOM	362	C	PRO	247	58.342	-8.431	11.325	1.00	61.94
ATOM	363	O	PRO	247	58.581	-7.256	11.053	1.00	61.60
ATOM	364	N	ALA	248	59.180	-9.219	11.990	1.00	61.33
ATOM	365	CA	ALA	248	60.468	-8.785	12.511	1.00	63.50
ATOM	366	CB	ALA	248	61.151	-9.991	13.174	1.00	66.94
ATOM	370	C	ALA	248	61.412	-8.140	11.489	1.00	64.19
ATOM	371	O	ALA	248	62.449	-7.593	11.867	1.00	65.56
ATOM	372	N	ASP	249	61.055	-8.188	10.207	1.00	64.36
ATOM	373	CA	ASP	249	61.900	-7.610	9.163	1.00	63.33
ATOM	374	CB	ASP	249	62.104	-8.618	8.026	1.00	62.97
ATOM	375	CG	ASP	249	60.798	-9.051	7.395	1.00	64.63
ATOM	376	OD1	ASP	249	60.037	-9.803	8.043	1.00	64.

ATOM	377	OD2	ASP	249	60.526	-8.626	6.253	1.00	66.52
ATOM	378	C	ASP	249	61.388	-6.293	8.572	1.00	64.31
ATOM	379	O	ASP	249	62.112	-5.624	7.830	1.00	64.73
ATOM	380	N	ILE	250	60.148	-5.927	8.885	1.00	63.09
ATOM	381	CA	ILE	250	59.577	-4.676	8.385	1.00	64.39
ATOM	382	CB	ILE	250	58.035	-4.741	8.349	1.00	65.79
ATOM	383	CG2	ILE	250	57.463	-3.408	7.861	1.00	64.78
ATOM	384	CG1	ILE	250	57.594	-5.893	7.439	1.00	65.28
ATOM	385	CD1	ILE	250	56.094	-6.103	7.362	1.00	65.08
ATOM	386	C	ILE	250	60.015	-3.534	9.299	1.00	65.21
ATOM	387	O	ILE	250	60.002	-3.676	10.524	1.00	64.05
ATOM	388	N	GLY	251	60.401	-2.405	8.700	1.00	65.48
ATOM	389	CA	GLY	251	60.864	-1.263	9.472	1.00	67.32
ATOM	390	C	GLY	251	62.069	-1.711	10.271	1.00	68.52
ATOM	391	O	GLY	251	62.099	-1.610	11.497	1.00	65.49
ATOM	392	N	GLN	252	63.080	-2.194	9.555	1.00	72.26
ATOM	393	CA	GLN	252	64.277	-2.726	10.176	1.00	74.10
ATOM	394	CB	GLN	252	64.598	-4.068	9.515	1.00	75.82
ATOM	395	CG	GLN	252	65.518	-4.974	10.302	1.00	77.81
ATOM	396	CD	GLN	252	65.686	-6.319	9.630	1.00	79.38
ATOM	397	OE1	GLN	252	66.087	-6.397	8.468	1.00	80.55
ATOM	398	NE2	GLN	252	65.384	-7.391	10.357	1.00	78.12
ATOM	399	C	GLN	252	65.496	-1.817	10.138	1.00	77.17
ATOM	400	O	GLN	252	65.553	-0.826	9.399	1.00	76.50
ATOM	401	N	ALA	253	66.470	-2.187	10.966	1.00	80.78
ATOM	402	CA	ALA	253	67.729	-1.475	11.104	1.00	83.70
ATOM	403	CB	ALA	253	68.402	-1.903	12.401	1.00	83.23
ATOM	404	C	ALA	253	68.639	-1.774	9.913	1.00	85.59
ATOM	405	O	ALA	253	68.294	-2.673	9.117	1.00	85.69
ATOM	406	OXT	ALA	253	69.694	-1.115	9.802	1.00	88.37
ATOM	429	CB	LYS	263	65.708	7.766	4.514	1.00	63.50
ATOM	430	C	LYS	263	64.141	6.903	6.272	1.00	63.41
ATOM	431	O	LYS	263	64.442	5.776	6.673	1.00	61.93
ATOM	432	N	LYS	263	66.368	7.841	6.894	1.00	61.71
ATOM	433	CA	LYS	263	65.218	7.942	5.950	1.00	64.36
ATOM	434	N	VAL	264	62.886	7.305	6.090	1.00	61.15
ATOM	435	CA	VAL	264	61.724	6.462	6.351	1.00	59.46
ATOM	436	CB	VAL	264	60.429	7.221	5.962	1.00	59.03
ATOM	437	CG1	VAL	264	59.200	6.421	6.363	1.00	53.79
ATOM	438	CG2	VAL	264	60.422	8.593	6.623	1.00	55.32
ATOM	439	C	VAL	264	61.790	5.129	5.595	1.00	60.96
ATOM	440	O	VAL	264	62.071	5.098	4.395	1.00	62.13
ATOM	441	N	ASP	265	61.522	4.034	6.304	1.00	62.59
ATOM	442	CA	ASP	265	61.562	2.693	5.727	1.00	64.95
ATOM	443	CB	ASP	265	61.322	1.644	6.810	1.00	64.32
ATOM	444	CG	ASP	265	61.415	0.232	6.277	1.00	67.70

ATOM	445	OD1 ASP	265	62.514	-0.158	5.831	1.00	72.59
ATOM	446	OD2 ASP	265	60.393	-0.486	6.289	1.00	68.84
ATOM	447	C ASP	265	60.560	2.470	4.591	1.00	65.64
ATOM	448	O ASP	265	60.789	1.637	3.717	1.00	68.81
ATOM	449	N LEU	266	59.456	3.211	4.624	1.00	65.12
ATOM	450	CA LEU	266	58.394	3.138	3.615	1.00	63.40
ATOM	451	CB LEU	266	58.963	3.333	2.202	1.00	67.34
ATOM	452	CG LEU	266	59.665	4.662	1.894	1.00	69.35
ATOM	453	CD1 LEU	266	60.193	4.627	0.469	1.00	68.24
ATOM	454	CD2 LEU	266	58.705	5.831	2.075	1.00	70.47
ATOM	455	C LEU	266	57.562	1.854	3.658	1.00	59.67
ATOM	456	O LEU	266	56.342	1.903	3.486	1.00	53.35
ATOM	457	N GLU	267	58.205	0.713	3.872	1.00	58.01
ATOM	458	CA GLU	267	57.454	-0.535	3.945	1.00	58.34
ATOM	459	CB GLU	267	58.387	-1.750	3.921	1.00	59.21
ATOM	460	CG GLU	267	57.640	-3.072	4.053	1.00	62.89
ATOM	461	CD GLU	267	58.548	-4.285	3.979	1.00	67.66
ATOM	462	OE1 GLU	267	59.513	-4.371	4.771	1.00	69.95
ATOM	463	OE2 GLU	267	58.285	-5.162	3.129	1.00	69.40
ATOM	464	C GLU	267	56.666	-0.515	5.243	1.00	57.67
ATOM	465	O GLU	267	55.488	-0.877	5.276	1.00	58.34
ATOM	466	N ALA	268	57.327	-0.077	6.317	1.00	53.43
ATOM	467	CA ALA	268	56.701	0.013	7.629	1.00	49.00
ATOM	468	CB ALA	268	57.766	0.244	8.695	1.00	45.72
ATOM	469	C ALA	268	55.701	1.166	7.611	1.00	45.76
ATOM	470	O ALA	268	54.598	1.057	8.144	1.00	41.50
ATOM	471	N PHE	269	56.106	2.267	6.983	1.00	41.43
ATOM	472	CA PHE	269	55.277	3.457	6.855	1.00	43.96
ATOM	473	CB PHE	269	56.016	4.511	6.022	1.00	40.10
ATOM	474	CG PHE	269	55.264	5.818	5.859	1.00	40.44
ATOM	475	CD1 PHE	269	55.102	6.690	6.949	1.00	38.98
ATOM	476	CD2 PHE	269	54.706	6.170	4.626	1.00	37.15
ATOM	477	CE1 PHE	269	54.401	7.920	6.807	1.00	32.12
ATOM	478	CE2 PHE	269	53.999	7.389	4.457	1.00	38.41
ATOM	479	CZ PHE	269	53.843	8.269	5.554	1.00	40.55
ATOM	480	C PHE	269	53.976	3.081	6.151	1.00	49.76
ATOM	481	O PHE	269	52.903	3.622	6.443	1.00	52.15
ATOM	482	N SER	270	54.089	2.140	5.217	1.00	53.15
ATOM	483	CA SER	270	52.957	1.669	4.432	1.00	52.29
ATOM	484	CB SER	270	53.456	0.703	3.349	1.00	51.85
ATOM	485	OG SER	270	52.400	0.297	2.499	1.00	53.42
ATOM	486	C SER	270	51.901	0.992	5.303	1.00	49.38
ATOM	487	O SER	270	50.713	1.284	5.185	1.00	48.74
ATOM	488	N HIS	271	52.335	0.085	6.173	1.00	50.15
ATOM	489	CA HIS	271	51.410	-0.614	7.061	1.00	51.67
ATOM	490	CB HIS	271	52.150	-1.682	7.878	1.00	58.52

ATOM	491	CG	HIS	271	52.697	-2.808	7.059	1.00	68.97
ATOM	492	CD2	HIS	271	52.425	-4.131	7.063	1.00	70.88
ATOM	493	ND1	HIS	271	53.660	-2.621	6.080	1.00	71.98
ATOM	494	CE1	HIS	271	53.951	-3.782	5.528	1.00	73.91
ATOM	495	NE2	HIS	271	53.214	-4.720	6.104	1.00	73.59
ATOM	496	C -	HIS	271	50.711	0.365	8.008	1.00	48.33
ATOM	497	O	HIS	271	49.507	0.260	8.240	1.00	48.39
ATOM	498	N	PHE	272	51.472	1.321	8.537	1.00	41.34
ATOM	499	CA	PHE	272	50.946	2.316	9.462	1.00	39.44
ATOM	500	CB	PHE	272	52.076	3.215	9.976	1.00	36.67
ATOM	501	CG	PHE	272	53.167	2.475	10.749	1.00	33.39
ATOM	502	CD1	PHE	272	54.421	3.065	10.915	1.00	33.14
ATOM	503	CD2	PHE	272	52.934	1.216	11.311	1.00	38.28
ATOM	504	CE1	PHE	272	55.454	2.418	11.633	1.00	38.26
ATOM	505	CE2	PHE	272	53.961	0.538	12.047	1.00	43.28
ATOM	506	CZ	PHE	272	55.225	1.146	12.207	1.00	39.74
ATOM	507	C	PHE	272	49.857	3.183	8.822	1.00	40.75
ATOM	508	O	PHE	272	48.784	3.361	9.394	1.00	35.51
ATOM	509	N	THR	273	50.136	3.714	7.635	1.00	41.64
ATOM	510	CA	THR	273	49.170	4.561	6.938	1.00	45.97
ATOM	511	CB	THR	273	49.813	5.249	5.711	1.00	51.52
ATOM	512	OG1	THR	273	50.339	4.257	4.815	1.00	45.74
ATOM	513	CG2	THR	273	50.936	6.179	6.158	1.00	49.73
ATOM	514	C	THR	273	47.941	3.772	6.481	1.00	46.23
ATOM	515	O	THR	273	46.879	4.344	6.233	1.00	41.21
ATOM	516	N	LYS	274	48.090	2.455	6.380	1.00	46.21
ATOM	517	CA	LYS	274	46.984	1.608	5.955	1.00	54.53
ATOM	518	CB	LYS	274	47.482	0.180	5.708	1.00	54.36
ATOM	519	C	LYS	274	45.878	1.595	7.006	1.00	56.88
ATOM	520	O	LYS	274	44.695	1.486	6.675	1.00	57.98
ATOM	521	N	ILE	275	46.267	1.718	8.268	1.00	56.48
ATOM	522	CA	ILE	275	45.312	1.695	9.368	1.00	52.64
ATOM	523	CB	ILE	275	45.710	0.611	10.391	1.00	49.15
ATOM	524	CG2	ILE	275	45.719	-0.758	9.701	1.00	47.42
ATOM	525	CG1	ILE	275	47.101	0.921	10.971	1.00	45.31
ATOM	526	CD1	ILE	275	47.565	-0.050	12.053	1.00	37.22
ATOM	527	C	ILE	275	45.175	3.032	10.086	1.00	51.78
ATOM	528	O	ILE	275	44.578	3.108	11.159	1.00	49.80
ATOM	529	N	ILE	276	45.710	4.088	9.481	1.00	51.76
ATOM	530	CA	ILE	276	45.657	5.416	10.084	1.00	52.58
ATOM	531	CB	ILE	276	46.733	6.364	9.464	1.00	55.04
ATOM	532	CG2	ILE	276	46.395	6.696	8.020	1.00	53.28
ATOM	533	CG1	ILE	276	46.823	7.663	10.270	1.00	57.31
ATOM	534	CD1	ILE	276	47.364	7.485	11.664	1.00	60.32
ATOM	535	C	ILE	276	44.279	6.073	9.974	1.00	50.70
ATOM	536	O	ILE	276	43.858	6.775	10.895	1.00	55.55



ATOM	537	N	THR	277	43.576	5.849	8.866	1.00	47.33
ATOM	538	CA	THR	277	42.255	6.450	8.681	1.00	42.59
ATOM	539	CB	THR	277	41.695	6.190	7.254	1.00	44.97
ATOM	540	OG1	THR	277	42.611	6.702	6.280	1.00	46.38
ATOM	541	CG2	THR	277	40.349	6.892	7.065	1.00	37.17
ATOM	542	C-	THR	277	41.252	5.954	9.718	1.00	39.84
ATOM	543	O	THR	277	40.570	6.759	10.351	1.00	40.55
ATOM	544	N	PRO	278	41.126	4.620	9.899	1.00	38.20
ATOM	545	CD	PRO	278	41.746	3.457	9.242	1.00	36.34
ATOM	546	CA	PRO	278	40.165	4.167	10.907	1.00	36.63
ATOM	547	CB	PRO	278	40.242	2.639	10.783	1.00	32.95
ATOM	548	CG	PRO	278	41.668	2.419	10.343	1.00	35.75
ATOM	549	C	PRO	278	40.532	4.681	12.306	1.00	38.60
ATOM	550	O	PRO	278	39.653	5.017	13.104	1.00	37.67
ATOM	551	N	ALA	279	41.831	4.758	12.586	1.00	37.05
ATOM	552	CA	ALA	279	42.315	5.248	13.877	1.00	33.18
ATOM	553	CB	ALA	279	43.836	5.135	13.949	1.00	30.56
ATOM	554	C	ALA	279	41.890	6.692	14.077	1.00	33.47
ATOM	555	O	ALA	279	41.403	7.060	15.151	1.00	33.74
ATOM	556	N	ILE	280	42.067	7.517	13.041	1.00	29.96
ATOM	557	CA	ILE	280	41.687	8.921	13.121	1.00	25.94
ATOM	558	CB	ILE	280	42.155	9.716	11.871	1.00	26.95
ATOM	559	CG2	ILE	280	41.643	11.168	11.923	1.00	15.40
ATOM	560	CG1	ILE	280	43.686	9.702	11.798	1.00	26.73
ATOM	561	CD1	ILE	280	44.255	10.378	10.550	1.00	34.31
ATOM	562	C	ILE	280	40.181	9.074	13.251	1.00	31.39
ATOM	563	O	ILE	280	39.696	9.943	13.973	1.00	35.69
ATOM	564	N	THR	281	39.428	8.226	12.552	1.00	30.90
ATOM	565	CA	THR	281	37.982	8.318	12.592	1.00	33.49
ATOM	566	CB	THR	281	37.321	7.451	11.478	1.00	37.18
ATOM	567	OG1	THR	281	37.760	6.091	11.592	1.00	46.48
ATOM	568	CG2	THR	281	37.703	7.972	10.114	1.00	32.85
ATOM	569	C	THR	281	37.435	7.926	13.968	1.00	29.94
ATOM	570	O	THR	281	36.428	8.473	14.408	1.00	25.55
ATOM	571	N	ARG	282	38.103	6.997	14.641	1.00	32.70
ATOM	572	CA	ARG	282	37.676	6.585	15.975	1.00	34.27
ATOM	573	CB	ARG	282	38.511	5.411	16.479	1.00	33.78
ATOM	574	CG	ARG	282	38.259	4.111	15.743	1.00	45.15
ATOM	575	CD	ARG	282	39.017	2.976	16.404	1.00	58.24
ATOM	576	NE	ARG	282	38.763	1.679	15.776	1.00	68.41
ATOM	577	CZ	ARG	282	39.141	1.344	14.546	1.00	72.31
ATOM	578	NH1	ARG	282	39.802	2.213	13.791	1.00	77.89
ATOM	579	NH2	ARG	282	38.864	0.139	14.066	1.00	69.25
ATOM	580	C	ARG	282	37.789	7.764	16.942	1.00	34.81
ATOM	581	O	ARG	282	37.006	7.886	17.884	1.00	36.03
ATOM	582	N	VAL	283	38.761	8.640	16.696	1.00	31.71



ATOM	583	CA	VAL	283	38.952	9.815	17.532	1.00	30.16
ATOM	584	CB	VAL	283	40.298	10.524	17.224	1.00	29.00
ATOM	585	CG1	VAL	283	40.448	11.777	18.076	1.00	28.64
ATOM	586	CG2	VAL	283	41.448	9.577	17.487	1.00	28.28
ATOM	587	C	VAL	283	37.801	10.787	17.292	1.00	32.50
ATOM	588	O.	VAL	283	37.284	11.388	18.236	1.00	33.48
ATOM	589	N	VAL	284	37.403	10.945	16.028	1.00	30.96
ATOM	590	CA	VAL	284	36.293	11.838	15.694	1.00	29.14
ATOM	591	CB	VAL	284	36.138	12.023	14.158	1.00	31.27
ATOM	592	CG1	VAL	284	34.990	12.985	13.868	1.00	24.21
ATOM	593	CG2	VAL	284	37.450	12.565	13.554	1.00	30.51
ATOM	594	C	VAL	284	34.995	11.260	16.258	1.00	28.89
ATOM	595	O	VAL	284	34.146	12.005	16.743	1.00	27.29
ATOM	596	N	ASP	285	34.845	9.937	16.208	1.00	28.76
ATOM	597	CA	ASP	285	33.639	9.307	16.738	1.00	35.32
ATOM	598	CB	ASP	285	33.627	7.792	16.459	1.00	33.29
ATOM	599	CG	ASP	285	33.523	7.471	14.971	1.00	38.15
ATOM	600	OD1	ASP	285	32.729	8.139	14.276	1.00	34.70
ATOM	601	OD2	ASP	285	34.209	6.532	14.504	1.00	34.43
ATOM	602	C	ASP	285	33.531	9.553	18.248	1.00	36.70
ATOM	603	O	ASP	285	32.431	9.685	18.786	1.00	37.96
ATOM	604	N	PHE	286	34.679	9.624	18.916	1.00	35.96
ATOM	605	CA	PHE	286	34.736	9.869	20.349	1.00	37.10
ATOM	606	CB	PHE	286	36.187	9.777	20.845	1.00	37.97
ATOM	607	CG	PHE	286	36.377	10.219	22.283	1.00	36.50
ATOM	608	CD1	PHE	286	35.815	9.490	23.340	1.00	36.75
ATOM	609	CD2	PHE	286	37.100	11.381	22.575	1.00	33.83
ATOM	610	CE1	PHE	286	35.966	9.917	24.685	1.00	39.55
ATOM	611	CE2	PHE	286	37.265	11.831	23.911	1.00	38.08
ATOM	612	CZ	PHE	286	36.696	11.092	24.972	1.00	34.44
ATOM	613	C	PHE	286	34.179	11.249	20.665	1.00	36.83
ATOM	614	O	PHE	286	33.292	11.401	21.518	1.00	35.61
ATOM	615	N	ALA	287	34.696	12.255	19.968	1.00	37.33
ATOM	616	CA	ALA	287	34.266	13.631	20.171	1.00	36.34
ATOM	617	CB	ALA	287	35.118	14.565	19.325	1.00	36.40
ATOM	618	C	ALA	287	32.785	13.840	19.861	1.00	38.76
ATOM	619	O	ALA	287	32.121	14.641	20.525	1.00	41.98
ATOM	620	N	LYS	288	32.267	13.130	18.862	1.00	38.28
ATOM	621	CA	LYS	288	30.856	13.268	18.499	1.00	45.26
ATOM	622	CB	LYS	288	30.541	12.534	17.188	1.00	48.35
ATOM	623	CG	LYS	288	31.159	13.158	15.951	1.00	51.43
ATOM	624	CD	LYS	288	30.556	12.589	14.665	1.00	60.23
ATOM	625	CE	LYS	288	30.848	11.107	14.479	1.00	62.81
ATOM	626	NZ	LYS	288	32.312	10.852	14.392	1.00	64.69
ATOM	627	C	LYS	288	29.913	12.763	19.586	1.00	43.31
ATOM	628	O	LYS	288	28.791	13.253			

ATOM	629	N	LYS	289	30.367	11.789	20.371	1.00	41.70
ATOM	630	CA	LYS	289	29.548	11.235	21.443	1.00	40.67
ATOM	631	CB	LYS	289	29.984	9.806	21.767	1.00	42.25
ATOM	632	CG	LYS	289	29.912	8.853	20.591	1.00	39.53
ATOM	633	CD	LYS	289	30.341	7.456	21.003	1.00	43.19
ATOM	634	CE	LYS	289	30.454	6.539	19.807	1.00	45.74
ATOM	635	NZ	LYS	289	29.175	6.457	19.049	1.00	52.49
ATOM	636	C	LYS	289	29.585	12.076	22.721	1.00	41.50
ATOM	637	O	LYS	289	29.030	11.676	23.742	1.00	39.77
ATOM	638	N	LEU	290	30.242	13.235	22.661	1.00	40.68
ATOM	639	CA	LEU	290	30.307	14.143	23.811	1.00	39.33
ATOM	640	CB	LEU	290	31.757	14.590	24.075	1.00	36.14
ATOM	641	CG	LEU	290	32.815	13.526	24.401	1.00	34.81
ATOM	642	CD1	LEU	290	34.155	14.200	24.558	1.00	29.07
ATOM	643	CD2	LEU	290	32.445	12.764	25.667	1.00	33.45
ATOM	644	C	LEU	290	29.448	15.368	23.481	1.00	40.08
ATOM	645	O	LEU	290	29.828	16.196	22.655	1.00	42.00
ATOM	646	N	PRO	291	28.279	15.500	24.137	1.00	40.27
ATOM	647	CD	PRO	291	27.716	14.625	25.185	1.00	39.65
ATOM	648	CA	PRO	291	27.372	16.628	23.899	1.00	38.28
ATOM	649	CB	PRO	291	26.327	16.447	24.997	1.00	35.88
ATOM	650	CG	PRO	291	26.230	14.932	25.071	1.00	34.19
ATOM	651	C	PRO	291	28.010	18.006	23.910	1.00	40.05
ATOM	652	O	PRO	291	27.663	18.857	23.089	1.00	41.33
ATOM	653	N	MET	292	28.933	18.235	24.837	1.00	40.59
ATOM	654	CA	MET	292	29.607	19.529	24.932	1.00	42.86
ATOM	655	CB	MET	292	30.635	19.521	26.059	1.00	43.28
ATOM	656	CG	MET	292	30.050	19.286	27.428	1.00	50.35
ATOM	657	SD	MET	292	31.329	19.157	28.679	1.00	51.17
ATOM	658	CE	MET	292	30.331	18.787	30.111	1.00	54.63
ATOM	659	C	MET	292	30.311	19.869	23.629	1.00	41.05
ATOM	660	O	MET	292	30.341	21.024	23.210	1.00	39.66
ATOM	661	N	PHE	293	30.882	18.854	22.992	1.00	39.30
ATOM	662	CA	PHE	293	31.594	19.057	21.747	1.00	40.92
ATOM	663	CB	PHE	293	32.300	17.772	21.335	1.00	40.98
ATOM	664	CG	PHE	293	33.117	17.902	20.070	1.00	42.78
ATOM	665	CD1	PHE	293	34.272	18.692	20.046	1.00	44.40
ATOM	666	CD2	PHE	293	32.727	17.235	18.902	1.00	43.66
ATOM	667	CE1	PHE	293	35.051	18.823	18.865	1.00	39.83
ATOM	668	CE2	PHE	293	33.483	17.348	17.710	1.00	46.21
ATOM	669	CZ	PHE	293	34.654	18.147	17.693	1.00	45.18
ATOM	670	C	PHE	293	30.653	19.492	20.624	1.00	45.54
ATOM	671	O	PHE	293	30.985	20.377	19.829	1.00	42.01
ATOM	672	N	CYS	294	29.468	18.895	20.579	1.00	47.05
ATOM	673	CA	CYS	294	28.545	19.200	19.512	1.00	50.15
ATOM	674	CB	CYS	294	27.3				

ATOM	675	SG	CYS	294	27.680	16.529	19.352	1.00	51.50
ATOM	676	C	CYS	294	28.062	20.636	19.582	1.00	51.38
ATOM	677	O	CYS	294	27.682	21.199	18.543	1.00	53.83
ATOM	678	N	GLU	295	27.996	21.170	20.802	1.00	49.72
ATOM	679	CA	GLU	295	27.541	22.535	21.067	1.00	52.53
ATOM	680	CB	GLU	295	27.384	22.762	22.575	1.00	57.40
ATOM	681	CG	GLU	295	26.179	22.090	23.208	1.00	69.63
ATOM	682	CD	GLU	295	24.871	22.731	22.785	1.00	78.49
ATOM	683	OE1	GLU	295	24.698	23.942	23.041	1.00	82.82
ATOM	684	OE2	GLU	295	24.017	22.029	22.199	1.00	85.30
ATOM	685	C	GLU	295	28.484	23.589	20.515	1.00	48.54
ATOM	686	O	GLU	295	28.170	24.777	20.537	1.00	49.82
ATOM	687	N	LEU	296	29.637	23.149	20.030	1.00	43.79
ATOM	688	CA	LEU	296	30.629	24.066	19.476	1.00	45.42
ATOM	689	CB	LEU	296	32.040	23.541	19.771	1.00	41.04
ATOM	690	CG	LEU	296	32.416	23.394	21.252	1.00	42.74
ATOM	691	CD1	LEU	296	33.789	22.753	21.352	1.00	40.99
ATOM	692	CD2	LEU	296	32.406	24.755	21.945	1.00	39.44
ATOM	693	C	LEU	296	30.448	24.239	17.968	1.00	45.56
ATOM	694	O	LEU	296	29.966	23.333	17.278	1.00	43.07
ATOM	695	N	PRO	297	30.823	25.414	17.436	1.00	46.99
ATOM	696	CD	PRO	297	31.372	26.613	18.083	1.00	47.12
ATOM	697	CA	PRO	297	30.689	25.650	15.998	1.00	49.61
ATOM	698	CB	PRO	297	31.106	27.118	15.861	1.00	49.91
ATOM	699	CG	PRO	297	30.757	27.693	17.230	1.00	51.28
ATOM	700	C	PRO	297	31.600	24.717	15.202	1.00	49.59
ATOM	701	O	PRO	297	32.727	24.446	15.615	1.00	51.66
ATOM	702	N	CYS	298	31.093	24.227	14.075	1.00	51.02
ATOM	703	CA	CYS	298	31.817	23.322	13.158	1.00	52.86
ATOM	704	CB	CYS	298	31.100	23.260	11.804	1.00	54.57
ATOM	705	SG	CYS	298	31.935	24.249	10.470	1.00	67.87
ATOM	706	C	CYS	298	33.269	23.797	12.974	1.00	48.51
ATOM	707	O	CYS	298	34.197	22.991	12.819	1.00	49.58
ATOM	708	N	GLU	299	33.464	25.113	13.019	1.00	44.17
ATOM	709	CA	GLU	299	34.797	25.692	12.890	1.00	47.57
ATOM	710	CB	GLU	299	34.741	27.227	12.912	1.00	49.92
ATOM	711	CG	GLU	299	34.001	27.871	11.747	1.00	59.30
ATOM	712	CD	GLU	299	32.489	27.763	11.848	1.00	63.80
ATOM	713	OE1	GLU	299	31.805	28.162	10.882	1.00	69.03
ATOM	714	OE2	GLU	299	31.979	27.297	12.889	1.00	67.10
ATOM	715	C	GLU	299	35.698	25.213	14.031	1.00	46.57
ATOM	716	O	GLU	299	36.772	24.659	13.787	1.00	44.65
ATOM	717	N	ASP	300	35.263	25.432	15.274	1.00	45.17
ATOM	718	CA	ASP	300	36.046	25.008	16.433	1.00	43.32
ATOM	719	CB	ASP	300	35.442	25.517	17.747	1.00	37.38
ATOM	720	CG	ASP						

ATOM	721	OD1 ASP	300	36.486	27.613	17.313	1.00	35.87
ATOM	722	OD2 ASP	300	34.769	27.601	18.669	1.00	40.14
ATOM	723	C ASP	300	36.174	23.495	16.513	1.00	42.81
ATOM	724	O ASP	300	37.193	22.979	16.974	1.00	46.02
ATOM	725	N GLN	301	35.139	22.788	16.066	1.00	38.60
ATOM	726	CA GLN	301	35.151	21.334	16.086	1.00	40.00
ATOM	727	CB GLN	301	33.815	20.783	15.576	1.00	38.59
ATOM	728	CG GLN	301	32.608	21.334	16.317	1.00	40.26
ATOM	729	CD GLN	301	31.311	20.696	15.869	1.00	44.15
ATOM	730	OE1 GLN	301	31.074	20.527	14.673	1.00	45.73
ATOM	731	NE2 GLN	301	30.450	20.363	16.824	1.00	46.13
ATOM	732	C GLN	301	36.298	20.807	15.227	1.00	41.64
ATOM	733	O GLN	301	36.975	19.850	15.601	1.00	45.02
ATOM	734	N ILE	302	36.523	21.441	14.077	1.00	41.01
ATOM	735	CA ILE	302	37.607	21.029	13.189	1.00	40.23
ATOM	736	CB ILE	302	37.580	21.798	11.825	1.00	39.52
ATOM	737	CG2 ILE	302	38.724	21.308	10.931	1.00	31.98
ATOM	738	CG1 ILE	302	36.230	21.607	11.119	1.00	40.77
ATOM	739	CD1 ILE	302	35.895	20.166	10.733	1.00	45.43
ATOM	740	C ILE	302	38.948	21.322	13.869	1.00	38.58
ATOM	741	O ILE	302	39.811	20.452	13.938	1.00	40.81
ATOM	742	N ILE	303	39.110	22.547	14.364	1.00	37.50
ATOM	743	CA ILE	303	40.343	22.958	15.030	1.00	39.33
ATOM	744	CB ILE	303	40.263	24.442	15.501	1.00	39.06
ATOM	745	CG2 ILE	303	41.525	24.822	16.279	1.00	36.19
ATOM	746	CG1 ILE	303	40.103	25.358	14.280	1.00	40.15
ATOM	747	CD1 ILE	303	39.972	26.846	14.602	1.00	36.93
ATOM	748	C ILE	303	40.676	22.061	16.222	1.00	36.49
ATOM	749	O ILE	303	41.818	21.623	16.378	1.00	36.58
ATOM	750	N LEU	304	39.674	21.788	17.057	1.00	32.91
ATOM	751	CA LEU	304	39.851	20.940	18.234	1.00	27.55
ATOM	752	CB LEU	304	38.546	20.875	19.026	1.00	22.35
ATOM	753	CG LEU	304	38.472	21.629	20.361	1.00	26.88
ATOM	754	CD1 LEU	304	39.096	22.998	20.275	1.00	24.82
ATOM	755	CD2 LEU	304	37.024	21.728	20.787	1.00	23.69
ATOM	756	C LEU	304	40.313	19.534	17.855	1.00	28.05
ATOM	757	O LEU	304	41.277	19.013	18.429	1.00	24.68
ATOM	758	N LEU	305	39.637	18.929	16.882	1.00	26.34
ATOM	759	CA LEU	305	39.997	17.588	16.436	1.00	30.91
ATOM	760	CB LEU	305	38.937	17.055	15.466	1.00	32.50
ATOM	761	CG LEU	305	37.585	16.757	16.132	1.00	33.36
ATOM	762	CD1 LEU	305	36.557	16.439	15.079	1.00	33.87
ATOM	763	CD2 LEU	305	37.733	15.581	17.101	1.00	31.72
ATOM	764	C LEU	305	41.381	17.523	15.796	1.00	29.76
ATOM	765	O LEU	305	42.109	16.553	15.990	1.00	29.33
ATOM	766	N LYS	306	41.754	18.554	15.048	1.00	29.72



ATOM	767	CA	LYS	306	43.065	18.569	14.409	1.00	34.28
ATOM	768	CB	LYS	306	43.122	19.673	13.345	1.00	35.98
ATOM	769	CG	LYS	306	42.140	19.465	12.206	1.00	43.35
ATOM	770	CD	LYS	306	42.195	20.583	11.170	1.00	51.50
ATOM	771	CE	LYS	306	43.532	20.639	10.446	1.00	53.26
ATOM	772	NZ	LYS	306	43.522	21.702	9.409	1.00	59.61
ATOM	773	C	LYS	306	44.183	18.777	15.434	1.00	35.25
ATOM	774	O	LYS	306	45.312	18.332	15.231	1.00	33.95
ATOM	775	N	GLY	307	43.853	19.446	16.536	1.00	35.79
ATOM	776	CA	GLY	307	44.836	19.700	17.576	1.00	34.59
ATOM	777	C	GLY	307	45.075	18.562	18.559	1.00	33.80
ATOM	778	O	GLY	307	46.200	18.360	19.008	1.00	31.59
ATOM	779	N	CYS	308	44.030	17.806	18.880	1.00	31.15
ATOM	780	CA	CYS	308	44.153	16.712	19.839	1.00	29.04
ATOM	781	CB	CYS	308	42.929	16.667	20.750	1.00	27.59
ATOM	782	SG	CYS	308	41.452	15.974	19.941	1.00	30.50
ATOM	783	C	CYS	308	44.289	15.339	19.208	1.00	30.59
ATOM	784	O	CYS	308	44.609	14.374	19.899	1.00	33.77
ATOM	785	N	CYS	309	44.053	15.247	17.907	1.00	28.46
ATOM	786	CA	CYS	309	44.099	13.961	17.219	1.00	30.10
ATOM	787	CB	CYS	309	43.983	14.161	15.706	1.00	33.43
ATOM	788	SG	CYS	309	43.761	12.613	14.819	1.00	35.20
ATOM	789	C	CYS	309	45.301	13.071	17.524	1.00	27.72
ATOM	790	O	CYS	309	45.135	11.907	17.913	1.00	27.69
ATOM	791	N	MET	310	46.508	13.594	17.339	1.00	26.15
ATOM	792	CA	MET	310	47.700	12.798	17.605	1.00	26.06
ATOM	793	CB	MET	310	48.928	13.439	16.951	1.00	25.32
ATOM	794	CG	MET	310	50.207	12.648	17.132	1.00	24.08
ATOM	795	SD	MET	310	50.101	10.991	16.423	1.00	27.71
ATOM	796	CE	MET	310	51.674	10.307	16.934	1.00	28.50
ATOM	797	C	MET	310	47.941	12.612	19.113	1.00	25.94
ATOM	798	O	MET	310	48.592	11.653	19.526	1.00	28.09
ATOM	799	N	GLU	311	47.405	13.522	19.923	1.00	25.39
ATOM	800	CA	GLU	311	47.560	13.445	21.370	1.00	27.03
ATOM	801	CB	GLU	311	47.099	14.748	22.030	1.00	24.39
ATOM	802	CG	GLU	311	47.610	15.999	21.331	1.00	26.00
ATOM	803	CD	GLU	311	47.292	17.271	22.084	1.00	23.95
ATOM	804	OE1	GLU	311	46.182	17.379	22.640	1.00	19.72
ATOM	805	OE2	GLU	311	48.150	18.181	22.088	1.00	26.51
ATOM	806	C	GLU	311	46.727	12.272	21.902	1.00	27.51
ATOM	807	O	GLU	311	47.152	11.552	22.807	1.00	29.67
ATOM	808	N	ILE	312	45.547	12.086	21.326	1.00	26.82
ATOM	809	CA	ILE	312	44.661	11.001	21.724	1.00	25.71
ATOM	810	CB	ILE	312	43.194	11.296	21.304	1.00	23.35
ATOM	811	CG2	ILE	312	42.301	10.068	21.583	1.00	20.27
ATOM	812	CG1	ILE	312					



ATOM	813	CD1	ILE	312	41.244	12.961	21.755	1.00	18.15
ATOM	814	C	ILE	312	45.116	9.665	21.132	1.00	27.91
ATOM	815	O	ILE	312	45.064	8.628	21.804	1.00	28.96
ATOM	816	N	MET	313	45.582	9.683	19.886	1.00	27.66
ATOM	817	CA	MET	313	46.045	8.447	19.257	1.00	30.18
ATOM	818	CB	MET	313	46.386	8.662	17.771	1.00	36.89
ATOM	819	CG	MET	313	45.186	8.938	16.861	1.00	37.95
ATOM	820	SD	MET	313	45.624	8.943	15.096	1.00	42.38
ATOM	821	CE	MET	313	46.724	10.319	14.999	1.00	40.68
ATOM	822	C	MET	313	47.264	7.897	19.975	1.00	27.43
ATOM	823	O	MET	313	47.351	6.690	20.219	1.00	28.61
ATOM	824	N	SER	314	48.202	8.776	20.318	1.00	24.88
ATOM	825	CA	SER	314	49.416	8.352	21.011	1.00	27.98
ATOM	826	CB	SER	314	50.420	9.511	21.118	1.00	29.64
ATOM	827	OG	SER	314	49.912	10.560	21.911	1.00	43.44
ATOM	828	C	SER	314	49.082	7.818	22.402	1.00	22.30
ATOM	829	O	SER	314	49.737	6.895	22.892	1.00	24.18
ATOM	830	N	LEU	315	48.070	8.395	23.039	1.00	23.99
ATOM	831	CA	LEU	315	47.646	7.918	24.365	1.00	25.07
ATOM	832	CB	LEU	315	46.580	8.842	24.965	1.00	19.11
ATOM	833	CG	LEU	315	45.863	8.355	26.228	1.00	20.39
ATOM	834	CD1	LEU	315	46.872	8.076	27.362	1.00	18.92
ATOM	835	CD2	LEU	315	44.848	9.401	26.655	1.00	12.93
ATOM	836	C	LEU	315	47.070	6.518	24.222	1.00	24.53
ATOM	837	O	LEU	315	47.394	5.615	24.992	1.00	26.32
ATOM	838	N	ARG	316	46.212	6.338	23.220	1.00	28.18
ATOM	839	CA	ARG	316	45.595	5.041	22.978	1.00	27.54
ATOM	840	CB	ARG	316	44.575	5.155	21.848	1.00	27.39
ATOM	841	CG	ARG	316	43.340	5.929	22.253	1.00	22.00
ATOM	842	CD	ARG	316	42.291	5.902	21.172	1.00	18.78
ATOM	843	NE	ARG	316	40.975	6.205	21.719	1.00	26.57
ATOM	844	CZ	ARG	316	39.852	6.224	21.014	1.00	30.81
ATOM	845	NH1	ARG	316	39.878	5.972	19.711	1.00	33.71
ATOM	846	NH2	ARG	316	38.692	6.471	21.613	1.00	33.13
ATOM	847	C	ARG	316	46.612	3.949	22.682	1.00	28.09
ATOM	848	O	ARG	316	46.399	2.790	23.027	1.00	32.41
ATOM	849	N	ALA	317	47.718	4.317	22.047	1.00	28.36
ATOM	850	CA	ALA	317	48.771	3.359	21.744	1.00	26.64
ATOM	851	CB	ALA	317	49.674	3.904	20.643	1.00	22.93
ATOM	852	C	ALA	317	49.591	3.115	23.002	1.00	28.35
ATOM	853	O	ALA	317	49.968	1.979	23.312	1.00	32.10
ATOM	854	N	ALA	318	49.863	4.197	23.727	1.00	29.12
ATOM	855	CA	ALA	318	50.655	4.123	24.953	1.00	27.50
ATOM	856	CB	ALA	318	50.854	5.518	25.522	1.00	28.39
ATOM	857	C	ALA	318	50.053	3.215	26.013	1.00	28.10
ATOM	858	O	ALA	318	50.783	2.491	26.684	1.00	28.18

ATOM	859	N	VAL	319	48.730	3.245	26.165	1.00	29.16
ATOM	860	CA	VAL	319	48.082	2.414	27.176	1.00	35.24
ATOM	861	CB	VAL	319	46.663	2.933	27.541	1.00	27.34
ATOM	862	CG1	VAL	319	46.759	4.324	28.136	1.00	29.96
ATOM	863	CG2	VAL	319	45.773	2.936	26.322	1.00	31.70
ATOM	864	C-	VAL	319	47.970	0.955	26.764	1.00	40.01
ATOM	865	O	VAL	319	47.448	0.129	27.515	1.00	42.70
ATOM	866	N	ARG	320	48.460	0.644	25.565	1.00	38.64
ATOM	867	CA	ARG	320	48.436	-0.715	25.041	1.00	38.61
ATOM	868	CB	ARG	320	47.764	-0.751	23.674	1.00	37.26
ATOM	869	CG	ARG	320	46.258	-0.655	23.720	1.00	43.12
ATOM	870	CD	ARG	320	45.712	-0.368	22.339	1.00	50.79
ATOM	871	NE	ARG	320	44.260	-0.446	22.286	1.00	54.71
ATOM	872	CZ	ARG	320	43.527	0.074	21.306	1.00	57.89
ATOM	873	NH1	ARG	320	44.119	0.713	20.300	1.00	49.08
ATOM	874	NH2	ARG	320	42.206	-0.058	21.326	1.00	59.59
ATOM	875	C	ARG	320	49.852	-1.247	24.930	1.00	42.14
ATOM	876	O	ARG	320	50.162	-2.055	24.051	1.00	46.30
ATOM	877	N	TYR	321	50.712	-0.772	25.822	1.00	42.04
ATOM	878	CA	TYR	321	52.098	-1.202	25.852	1.00	42.70
ATOM	879	CB	TYR	321	52.971	-0.133	26.529	1.00	38.01
ATOM	880	CG	TYR	321	54.416	-0.579	26.734	1.00	37.94
ATOM	881	CD1	TYR	321	55.275	-0.779	25.636	1.00	33.85
ATOM	882	CE1	TYR	321	56.581	-1.297	25.813	1.00	34.49
ATOM	883	CD2	TYR	321	54.892	-0.894	28.016	1.00	28.03
ATOM	884	CE2	TYR	321	56.194	-1.411	28.207	1.00	32.69
ATOM	885	CZ	TYR	321	57.026	-1.614	27.103	1.00	35.18
ATOM	886	OH	TYR	321	58.289	-2.158	27.288	1.00	39.48
ATOM	887	C	TYR	321	52.189	-2.515	26.629	1.00	45.51
ATOM	888	O	TYR	321	51.571	-2.662	27.687	1.00	48.02
ATOM	889	N	ASP	322	52.945	-3.471	26.095	1.00	44.56
ATOM	890	CA	ASP	322	53.129	-4.764	26.753	1.00	45.86
ATOM	891	CB	ASP	322	52.697	-5.899	25.816	1.00	46.64
ATOM	892	C	ASP	322	54.606	-4.910	27.098	1.00	45.82
ATOM	893	O	ASP	322	55.434	-5.109	26.214	1.00	45.38
ATOM	894	N	PRO	323	54.962	-4.803	28.393	1.00	46.53
ATOM	895	CD	PRO	323	54.123	-4.541	29.572	1.00	47.16
ATOM	896	CA	PRO	323	56.366	-4.932	28.805	1.00	46.63
ATOM	897	CB	PRO	323	56.293	-4.667	30.308	1.00	43.95
ATOM	898	CG	PRO	323	54.926	-5.223	30.655	1.00	43.93
ATOM	899	C	PRO	323	56.993	-6.285	28.478	1.00	48.34
ATOM	900	O	PRO	323	58.217	-6.407	28.379	1.00	50.84
ATOM	901	N	GLU	324	56.149	-7.301	28.315	1.00	52.39
ATOM	902	CA	GLU	324	56.621	-8.646	28.005	1.00	55.85
ATOM	903	CB	GLU	324	55.453	-9.633	28.048	1.00	55.54
ATOM	904	C	GLU	324	57.283	-8.670	26.632	1.00	54.

ATOM	905	O	GLU	324	58.460	-9.013	26.502	1.00	59.81
ATOM	906	N	SER	325	56.522	-8.299	25.611	1.00	52.95
ATOM	907	CA	SER	325	57.021	-8.269	24.244	1.00	50.10
ATOM	908	CB	SER	325	55.889	-8.613	23.279	1.00	48.23
ATOM	909	OG	SER	325	54.788	-7.749	23.471	1.00	48.71
ATOM	910	C.	SER	325	57.608	-6.908	23.879	1.00	50.61
ATOM	911	O	SER	325	58.194	-6.743	22.808	1.00	52.19
ATOM	912	N	GLU	326	57.450	-5.939	24.786	1.00	45.64
ATOM	913	CA	GLU	326	57.938	-4.579	24.588	1.00	43.35
ATOM	914	CB	GLU	326	59.469	-4.562	24.587	1.00	42.74
ATOM	915	CG	GLU	326	60.053	-5.016	25.909	1.00	50.32
ATOM	916	CD	GLU	326	61.565	-5.067	25.907	1.00	56.34
ATOM	917	OE1	GLU	326	62.139	-5.407	26.966	1.00	59.31
ATOM	918	OE2	GLU	326	62.178	-4.774	24.856	1.00	55.74
ATOM	919	C	GLU	326	57.397	-3.993	23.291	1.00	40.23
ATOM	920	O	GLU	326	58.145	-3.474	22.465	1.00	40.44
ATOM	921	N	THR	327	56.080	-4.079	23.127	1.00	35.90
ATOM	922	CA	THR	327	55.427	-3.573	21.936	1.00	37.29
ATOM	923	CB	THR	327	54.983	-4.717	21.008	1.00	37.63
ATOM	924	OG1	THR	327	53.994	-5.503	21.674	1.00	38.12
ATOM	925	CG2	THR	327	56.165	-5.609	20.635	1.00	39.90
ATOM	926	C	THR	327	54.170	-2.780	22.282	1.00	39.49
ATOM	927	O	THR	327	53.603	-2.930	23.364	1.00	40.50
ATOM	928	N	LEU	328	53.758	-1.933	21.347	1.00	36.64
ATOM	929	CA	LEU	328	52.544	-1.136	21.480	1.00	37.73
ATOM	930	CB	LEU	328	52.791	0.340	21.127	1.00	37.78
ATOM	931	CG	LEU	328	53.667	1.257	21.982	1.00	36.26
ATOM	932	CD1	LEU	328	53.690	2.641	21.348	1.00	36.56
ATOM	933	CD2	LEU	328	53.101	1.351	23.396	1.00	39.85
ATOM	934	C	LEU	328	51.617	-1.722	20.431	1.00	37.27
ATOM	935	O	LEU	328	52.083	-2.233	19.410	1.00	34.96
ATOM	936	N	THR	329	50.314	-1.652	20.669	1.00	39.73
ATOM	937	CA	THR	329	49.368	-2.173	19.701	1.00	40.81
ATOM	938	CB	THR	329	48.401	-3.176	20.349	1.00	42.67
ATOM	939	OG1	THR	329	49.156	-4.271	20.896	1.00	42.52
ATOM	940	CG2	THR	329	47.425	-3.722	19.315	1.00	43.52
ATOM	941	C	THR	329	48.591	-1.034	19.058	1.00	44.31
ATOM	942	O	THR	329	47.825	-0.325	19.712	1.00	43.72
ATOM	943	N	LEU	330	48.822	-0.859	17.759	1.00	44.62
ATOM	944	CA	LEU	330	48.179	0.182	16.972	1.00	45.09
ATOM	945	CB	LEU	330	49.056	0.545	15.766	1.00	44.66
ATOM	946	CG	LEU	330	50.329	1.393	15.951	1.00	51.06
ATOM	947	CD1	LEU	330	51.195	0.890	17.095	1.00	48.58
ATOM	948	CD2	LEU	330	51.107	1.387	14.638	1.00	45.18
ATOM	949	C	LEU	330	46.802	-0.264	16.501	1.00	48.06
ATOM	950	O	LEU	330	46.634	-1.386	16.012	1.	

ATOM	951	N	ASN	331	45.826	0.618	16.663	1.00	52.20
ATOM	952	CA	ASN	331	44.450	0.363	16.257	1.00	54.41
ATOM	953	CB	ASN	331	44.370	0.353	14.731	1.00	54.94
ATOM	954	CG	ASN	331	42.970	0.603	14.219	1.00	60.35
ATOM	955	OD1	ASN	331	42.375	1.642	14.501	1.00	61.84
ATOM	956	ND2	ASN	331	42.438	-0.344	13.459	1.00	65.92
ATOM	957	C	ASN	331	43.940	-0.963	16.836	1.00	58.00
ATOM	958	O	ASN	331	42.985	-1.557	16.328	1.00	60.17
ATOM	959	N	GLY	332	44.590	-1.414	17.908	1.00	58.45
ATOM	960	CA	GLY	332	44.215	-2.658	18.556	1.00	58.55
ATOM	961	C	GLY	332	44.408	-3.880	17.680	1.00	59.79
ATOM	962	O	GLY	332	43.892	-4.953	17.993	1.00	61.32
ATOM	963	N	GLU	333	45.165	-3.725	16.597	1.00	60.28
ATOM	964	CA	GLU	333	45.408	-4.821	15.659	1.00	59.13
ATOM	965	CB	GLU	333	44.817	-4.478	14.293	1.00	62.40
ATOM	966	CG	GLU	333	43.345	-4.129	14.296	1.00	75.69
ATOM	967	CD	GLU	333	42.851	-3.731	12.917	1.00	80.41
ATOM	968	OE1	GLU	333	43.374	-2.740	12.359	1.00	79.98
ATOM	969	OE2	GLU	333	41.942	-4.412	12.392	1.00	83.81
ATOM	970	C	GLU	333	46.881	-5.146	15.452	1.00	57.18
ATOM	971	O	GLU	333	47.291	-6.301	15.545	1.00	57.50
ATOM	972	N	MET	334	47.663	-4.112	15.166	1.00	55.20
ATOM	973	CA	MET	334	49.085	-4.245	14.873	1.00	50.85
ATOM	974	CB	MET	334	49.416	-3.334	13.687	1.00	48.70
ATOM	975	CG	MET	334	50.844	-3.412	13.181	1.00	45.39
ATOM	976	SD	MET	334	51.159	-2.124	11.959	1.00	44.56
ATOM	977	CE	MET	334	49.908	-2.477	10.749	1.00	45.25
ATOM	978	C	MET	334	50.041	-3.941	16.026	1.00	51.59
ATOM	979	O	MET	334	50.104	-2.810	16.508	1.00	52.52
ATOM	980	N	ALA	335	50.796	-4.946	16.450	1.00	51.00
ATOM	981	CA	ALA	335	51.769	-4.787	17.527	1.00	48.98
ATOM	982	CB	ALA	335	51.850	-6.062	18.347	1.00	47.86
ATOM	983	C	ALA	335	53.136	-4.470	16.917	1.00	51.01
ATOM	984	O	ALA	335	53.655	-5.242	16.109	1.00	51.61
ATOM	985	N	VAL	336	53.718	-3.336	17.307	1.00	46.62
ATOM	986	CA	VAL	336	55.016	-2.926	16.783	1.00	42.35
ATOM	987	CB	VAL	336	54.876	-1.687	15.877	1.00	42.41
ATOM	988	CG1	VAL	336	53.963	-2.004	14.707	1.00	42.00
ATOM	989	CG2	VAL	336	54.313	-0.506	16.676	1.00	40.32
ATOM	990	C	VAL	336	56.023	-2.608	17.883	1.00	45.33
ATOM	991	O	VAL	336	55.650	-2.309	19.019	1.00	47.42
ATOM	992	N	THR	337	57.310	-2.678	17.541	1.00	41.60
ATOM	993	CA	THR	337	58.357	-2.381	18.508	1.00	39.69
ATOM	994	CB	THR	337	59.608	-3.259	18.296	1.00	41.35
ATOM	995	OG1	THR	337	60.168	-2.985	17.007	1.00	49.35
ATOM	996	CG2	THR	337	59.253	-4.734	18.392	1.00	40.38



ATOM	997	C	THR	337	58.777	-0.924	18.367	1.00	37.88
ATOM	998	O	THR	337	58.312	-0.218	17.473	1.00	34.06
ATOM	999	N	ARG	338	59.655	-0.489	19.268	1.00	37.61
ATOM	1000	CA	ARG	338	60.171	0.876	19.268	1.00	38.68
ATOM	1001	CB	ARG	338	61.177	1.041	20.424	1.00	35.95
ATOM	1002	CG	ARG	338	61.804	2.434	20.570	1.00	38.83
ATOM	1003	CD	ARG	338	62.791	2.462	21.749	1.00	35.88
ATOM	1004	NE	ARG	338	62.114	2.277	23.035	1.00	37.42
ATOM	1005	CZ	ARG	338	61.858	3.256	23.902	1.00	30.20
ATOM	1006	NH1	ARG	338	62.224	4.501	23.636	1.00	27.98
ATOM	1007	NH2	ARG	338	61.213	2.992	25.025	1.00	27.40
ATOM	1008	C	ARG	338	60.843	1.158	17.925	1.00	38.09
ATOM	1009	O	ARG	338	60.529	2.142	17.251	1.00	34.12
ATOM	1010	N	GLY	339	61.755	0.267	17.535	1.00	41.25
ATOM	1011	CA	GLY	339	62.475	0.416	16.282	1.00	41.35
ATOM	1012	C	GLY	339	61.594	0.463	15.046	1.00	41.23
ATOM	1013	O	GLY	339	61.811	1.288	14.159	1.00	38.30
ATOM	1014	N	GLN	340	60.594	-0.414	14.982	1.00	38.58
ATOM	1015	CA	GLN	340	59.704	-0.449	13.826	1.00	40.79
ATOM	1016	CB	GLN	340	58.757	-1.651	13.911	1.00	40.82
ATOM	1017	CG	GLN	340	59.450	-2.995	13.944	1.00	41.10
ATOM	1018	CD	GLN	340	58.468	-4.144	13.890	1.00	48.84
ATOM	1019	OE1	GLN	340	57.529	-4.208	14.679	1.00	50.53
ATOM	1020	NE2	GLN	340	58.685	-5.068	12.959	1.00	54.25
ATOM	1021	C	GLN	340	58.884	0.822	13.679	1.00	41.50
ATOM	1022	O	GLN	340	58.725	1.342	12.576	1.00	42.72
ATOM	1023	N	LEU	341	58.360	1.324	14.795	1.00	42.00
ATOM	1024	CA	LEU	341	57.546	2.532	14.775	1.00	38.10
ATOM	1025	CB	LEU	341	56.868	2.740	16.133	1.00	36.66
ATOM	1026	CG	LEU	341	55.886	3.914	16.267	1.00	39.94
ATOM	1027	CD1	LEU	341	54.711	3.741	15.311	1.00	34.98
ATOM	1028	CD2	LEU	341	55.389	3.989	17.700	1.00	40.95
ATOM	1029	C	LEU	341	58.404	3.743	14.423	1.00	36.37
ATOM	1030	O	LEU	341	57.980	4.620	13.668	1.00	37.89
ATOM	1031	N	LYS	342	59.616	3.777	14.969	1.00	33.29
ATOM	1032	CA	LYS	342	60.542	4.872	14.723	1.00	35.17
ATOM	1033	CB	LYS	342	61.801	4.687	15.582	1.00	34.97
ATOM	1034	CG	LYS	342	62.764	5.863	15.519	1.00	40.00
ATOM	1035	CD	LYS	342	63.868	5.739	16.555	1.00	34.48
ATOM	1036	CE	LYS	342	64.709	7.001	16.596	1.00	37.54
ATOM	1037	NZ	LYS	342	65.716	6.972	17.689	1.00	42.32
ATOM	1038	C	LYS	342	60.928	4.970	13.235	1.00	38.29
ATOM	1039	O	LYS	342	60.621	5.963	12.569	1.00	36.23
ATOM	1040	N	ASN	343	61.585	3.932	12.721	1.00	39.25
ATOM	1041	CA	ASN	343	62.014	3.903	11.328	1.00	40.19
ATOM	1042	CB	ASN						



ATOM	1043	CG	ASN	343	63.937	2.429	12.027	1.00	39.22
ATOM	1044	OD1	ASN	343	64.648	3.376	12.374	1.00	42.37
ATOM	1045	ND2	ASN	343	64.125	1.197	12.471	1.00	42.19
ATOM	1046	C	ASN	343	60.831	3.997	10.368	1.00	40.12
ATOM	1047	O	ASN	343	60.991	4.371	9.208	1.00	36.01
ATOM	1048	N	GLY	344	59.645	3.665	10.868	1.00	40.95
ATOM	1049	CA	GLY	344	58.439	3.721	10.057	1.00	39.25
ATOM	1050	C	GLY	344	57.947	5.131	9.772	1.00	38.26
ATOM	1051	O	GLY	344	56.971	5.308	9.044	1.00	35.69
ATOM	1052	N	GLY	345	58.604	6.135	10.359	1.00	35.89
ATOM	1053	CA	GLY	345	58.212	7.510	10.110	1.00	34.00
ATOM	1054	C	GLY	345	58.050	8.444	11.300	1.00	38.64
ATOM	1055	O	GLY	345	57.902	9.652	11.116	1.00	38.14
ATOM	1056	N	LEU	346	58.085	7.912	12.520	1.00	39.52
ATOM	1057	CA	LEU	346	57.904	8.761	13.692	1.00	36.05
ATOM	1058	CB	LEU	346	57.039	8.048	14.738	1.00	35.72
ATOM	1059	CG	LEU	346	55.561	7.864	14.371	1.00	34.89
ATOM	1060	CD1	LEU	346	54.850	7.132	15.494	1.00	44.09
ATOM	1061	CD2	LEU	346	54.903	9.213	14.146	1.00	34.84
ATOM	1062	C	LEU	346	59.189	9.264	14.339	1.00	33.52
ATOM	1063	O	LEU	346	59.171	10.257	15.066	1.00	35.58
ATOM	1064	N	GLY	347	60.299	8.595	14.067	1.00	30.47
ATOM	1065	CA	GLY	347	61.559	9.017	14.661	1.00	33.01
ATOM	1066	C	GLY	347	61.504	9.069	16.182	1.00	30.72
ATOM	1067	O	GLY	347	60.967	8.160	16.812	1.00	30.89
ATOM	1068	N	VAL	348	62.051	10.132	16.765	1.00	31.30
ATOM	1069	CA	VAL	348	62.084	10.291	18.221	1.00	31.27
ATOM	1070	CB	VAL	348	62.843	11.612	18.620	1.00	31.66
ATOM	1071	CG1	VAL	348	62.071	12.841	18.146	1.00	20.19
ATOM	1072	CG2	VAL	348	63.080	11.651	20.118	1.00	24.77
ATOM	1073	C	VAL	348	60.683	10.273	18.855	1.00	33.84
ATOM	1074	O	VAL	348	60.546	10.034	20.050	1.00	29.99
ATOM	1075	N	VAL	349	59.649	10.518	18.049	1.00	33.31
ATOM	1076	CA	VAL	349	58.270	10.495	18.538	1.00	32.23
ATOM	1077	CB	VAL	349	57.279	10.911	17.415	1.00	32.59
ATOM	1078	CG1	VAL	349	55.837	10.678	17.838	1.00	33.68
ATOM	1079	CG2	VAL	349	57.474	12.378	17.103	1.00	32.30
ATOM	1080	C	VAL	349	57.931	9.094	19.050	1.00	34.91
ATOM	1081	O	VAL	349	57.133	8.932	19.980	1.00	33.73
ATOM	1082	N	SER	350	58.551	8.081	18.444	1.00	32.81
ATOM	1083	CA	SER	350	58.335	6.704	18.853	1.00	30.10
ATOM	1084	CB	SER	350	59.041	5.746	17.904	1.00	24.95
ATOM	1085	OG	SER	350	58.943	4.417	18.387	1.00	23.16
ATOM	1086	C	SER	350	58.863	6.486	20.266	1.00	31.59
ATOM	1087	O	SER	350	58.207	5.845	21.086	1.00	37.62
ATOM	1088	N	ASP						

ATOM	1089	CA	ASP	351	60.652	6.863	21.867	1.00	29.82
ATOM	1090	CB	ASP	351	62.048	7.491	21.919	1.00	27.49
ATOM	1091	CG	ASP	351	63.030	6.806	21.000	1.00	30.22
ATOM	1092	OD1	ASP	351	63.411	7.412	19.974	1.00	32.61
ATOM	1093	OD2	ASP	351	63.422	5.661	21.301	1.00	30.02
ATOM	1094	C.	ASP	351	59.785	7.548	22.913	1.00	30.63
ATOM	1095	O	ASP	351	59.632	7.055	24.027	1.00	29.54
ATOM	1096	N	ALA	352	59.222	8.692	22.537	1.00	25.33
ATOM	1097	CA	ALA	352	58.390	9.464	23.432	1.00	28.59
ATOM	1098	CB	ALA	352	58.011	10.798	22.788	1.00	20.95
ATOM	1099	C	ALA	352	57.136	8.695	23.831	1.00	29.69
ATOM	1100	O	ALA	352	56.711	8.753	24.982	1.00	30.36
ATOM	1101	N	ILE	353	56.557	7.979	22.876	1.00	27.63
ATOM	1102	CA	ILE	353	55.345	7.227	23.129	1.00	27.55
ATOM	1103	CB	ILE	353	54.611	6.925	21.805	1.00	28.04
ATOM	1104	CG2	ILE	353	53.329	6.111	22.065	1.00	23.68
ATOM	1105	CG1	ILE	353	54.269	8.251	21.119	1.00	27.33
ATOM	1106	CD1	ILE	353	53.637	8.105	19.734	1.00	26.23
ATOM	1107	C	ILE	353	55.631	5.943	23.901	1.00	30.88
ATOM	1108	O	ILE	353	54.880	5.597	24.814	1.00	31.22
ATOM	1109	N	PHE	354	56.710	5.240	23.549	1.00	29.86
ATOM	1110	CA	PHE	354	57.056	4.022	24.275	1.00	31.08
ATOM	1111	CB	PHE	354	58.227	3.274	23.619	1.00	28.80
ATOM	1112	CG	PHE	354	57.799	2.322	22.523	1.00	28.80
ATOM	1113	CD1	PHE	354	57.330	2.804	21.292	1.00	30.96
ATOM	1114	CD2	PHE	354	57.811	0.939	22.749	1.00	29.45
ATOM	1115	CE1	PHE	354	56.864	1.909	20.281	1.00	27.12
ATOM	1116	CE2	PHE	354	57.354	0.026	21.761	1.00	25.19
ATOM	1117	CZ	PHE	354	56.879	0.518	20.521	1.00	28.09
ATOM	1118	C	PHE	354	57.398	4.349	25.721	1.00	29.17
ATOM	1119	O	PHE	354	57.001	3.625	26.631	1.00	32.62
ATOM	1120	N	ASP	355	58.133	5.438	25.925	1.00	23.86
ATOM	1121	CA	ASP	355	58.508	5.873	27.262	1.00	25.34
ATOM	1122	CB	ASP	355	59.434	7.083	27.180	1.00	21.41
ATOM	1123	CG	ASP	355	60.846	6.708	26.769	1.00	32.08
ATOM	1124	OD1	ASP	355	61.051	5.595	26.226	1.00	33.58
ATOM	1125	OD2	ASP	355	61.756	7.534	26.970	1.00	33.20
ATOM	1126	C	ASP	355	57.254	6.211	28.062	1.00	27.86
ATOM	1127	O	ASP	355	57.167	5.916	29.252	1.00	32.42
ATOM	1128	N	LEU	356	56.276	6.821	27.401	1.00	26.84
ATOM	1129	CA	LEU	356	55.031	7.164	28.066	1.00	28.66
ATOM	1130	CB	LEU	356	54.112	7.953	27.131	1.00	25.37
ATOM	1131	CG	LEU	356	52.787	8.427	27.742	1.00	27.61
ATOM	1132	CD1	LEU	356	53.056	9.452	28.842	1.00	25.43
ATOM	1133	CD2	LEU	356	51.924	9.057	26.667	1.00	27.49
ATOM	1134	C	LEU	356					

ATOM	1135	O	LEU	356	53.873	5.743	29.601	1.00	31.55
ATOM	1136	N	GLY	357	54.266	4.928	27.536	1.00	32.69
ATOM	1137	CA	GLY	357	53.621	3.652	27.787	1.00	29.87
ATOM	1138	C	GLY	357	54.239	2.884	28.939	1.00	33.12
ATOM	1139	O	GLY	357	53.524	2.268	29.732	1.00	29.41
ATOM	1140	N	MET	358	55.570	2.911	29.026	1.00	33.31
ATOM	1141	CA	MET	358	56.277	2.217	30.100	1.00	35.87
ATOM	1142	CB	MET	358	57.794	2.265	29.871	1.00	34.56
ATOM	1143	CG	MET	358	58.265	1.608	28.576	1.00	46.43
ATOM	1144	SD	MET	358	60.073	1.600	28.351	1.00	42.13
ATOM	1145	CE	MET	358	60.429	3.306	28.411	1.00	44.29
ATOM	1146	C	MET	358	55.948	2.884	31.434	1.00	33.26
ATOM	1147	O	MET	358	55.802	2.222	32.453	1.00	36.39
ATOM	1148	N	SER	359	55.825	4.202	31.398	1.00	33.31
ATOM	1149	CA	SER	359	55.533	4.998	32.580	1.00	34.39
ATOM	1150	CB	SER	359	55.859	6.463	32.303	1.00	30.84
ATOM	1151	OG	SER	359	55.487	7.265	33.404	1.00	47.14
ATOM	1152	C	SER	359	54.094	4.897	33.072	1.00	36.43
ATOM	1153	O	SER	359	53.833	5.073	34.260	1.00	35.46
ATOM	1154	N	LEU	360	53.165	4.617	32.156	1.00	36.74
ATOM	1155	CA	LEU	360	51.750	4.519	32.493	1.00	35.44
ATOM	1156	CB	LEU	360	50.889	4.817	31.263	1.00	34.16
ATOM	1157	CG	LEU	360	50.896	6.263	30.751	1.00	34.59
ATOM	1158	CD1	LEU	360	50.031	6.353	29.513	1.00	33.53
ATOM	1159	CD2	LEU	360	50.376	7.211	31.836	1.00	31.69
ATOM	1160	C	LEU	360	51.324	3.192	33.088	1.00	38.72
ATOM	1161	O	LEU	360	50.185	3.058	33.546	1.00	38.29
ATOM	1162	N	SER	361	52.227	2.214	33.080	1.00	40.96
ATOM	1163	CA	SER	361	51.938	0.897	33.636	1.00	45.67
ATOM	1164	CB	SER	361	53.131	-0.044	33.436	1.00	46.45
ATOM	1165	OG	SER	361	53.362	-0.296	32.061	1.00	51.81
ATOM	1166	C	SER	361	51.628	1.004	35.124	1.00	44.49
ATOM	1167	O	SER	361	50.724	0.337	35.630	1.00	46.67
ATOM	1168	N	SER	362	52.385	1.858	35.809	1.00	41.44
ATOM	1169	CA	SER	362	52.231	2.081	37.245	1.00	42.13
ATOM	1170	CB	SER	362	53.431	2.876	37.779	1.00	42.61
ATOM	1171	OG	SER	362	54.647	2.215	37.492	1.00	51.87
ATOM	1172	C	SER	362	50.951	2.832	37.610	1.00	38.41
ATOM	1173	O	SER	362	50.444	2.700	38.722	1.00	38.01
ATOM	1174	N	PHE	363	50.443	3.631	36.672	1.00	34.55
ATOM	1175	CA	PHE	363	49.232	4.404	36.906	1.00	32.96
ATOM	1176	CB	PHE	363	49.109	5.518	35.859	1.00	31.99
ATOM	1177	CG	PHE	363	50.093	6.659	36.058	1.00	29.97
ATOM	1178	CD1	PHE	363	49.667	7.872	36.594	1.00	30.61
ATOM	1179	CD2	PHE	363	51.445	6.501	35.731	1.00	32.02
ATOM	1180	CE1	PHE	363	50.579</				

ATOM	1181	CE2	PHE	363	52.376	7.552	35.934	1.00	30.91
ATOM	1182	CZ	PHE	363	51.938	8.777	36.473	1.00	29.33
ATOM	1183	C	PHE	363	47.973	3.554	36.916	1.00	30.52
ATOM	1184	O	PHE	363	46.971	3.947	37.491	1.00	32.19
ATOM	1185	N	ASN	364	48.036	2.384	36.283	1.00	33.51
ATOM	1186	CA	ASN	364	46.894	1.471	36.216	1.00	38.03
ATOM	1187	CB	ASN	364	46.754	0.711	37.539	1.00	42.32
ATOM	1188	CG	ASN	364	47.824	-0.361	37.713	1.00	53.11
ATOM	1189	OD1	ASN	364	47.815	-1.370	37.012	1.00	59.51
ATOM	1190	ND2	ASN	364	48.751	-0.138	38.639	1.00	55.95
ATOM	1191	C	ASN	364	45.574	2.161	35.871	1.00	31.89
ATOM	1192	O	ASN	364	44.587	2.027	36.588	1.00	30.28
ATOM	1193	N	LEU	365	45.561	2.883	34.751	1.00	27.62
ATOM	1194	CA	LEU	365	44.365	3.606	34.317	1.00	29.36
ATOM	1195	CB	LEU	365	44.738	4.627	33.240	1.00	27.54
ATOM	1196	CG	LEU	365	45.826	5.659	33.576	1.00	38.91
ATOM	1197	CD1	LEU	365	46.115	6.499	32.338	1.00	34.47
ATOM	1198	CD2	LEU	365	45.394	6.546	34.743	1.00	34.24
ATOM	1199	C	LEU	365	43.264	2.691	33.774	1.00	26.23
ATOM	1200	O	LEU	365	43.546	1.648	33.197	1.00	27.06
ATOM	1201	N	ASP	366	42.011	3.074	33.991	1.00	25.23
ATOM	1202	CA	ASP	366	40.892	2.307	33.462	1.00	26.07
ATOM	1203	CB	ASP	366	39.832	2.008	34.538	1.00	29.68
ATOM	1204	CG	ASP	366	39.337	3.253	35.261	1.00	35.74
ATOM	1205	OD1	ASP	366	39.438	4.371	34.717	1.00	36.78
ATOM	1206	OD2	ASP	366	38.803	3.100	36.378	1.00	41.23
ATOM	1207	C	ASP	366	40.274	3.100	32.305	1.00	27.70
ATOM	1208	O	ASP	366	40.748	4.191	31.975	1.00	31.94
ATOM	1209	N	ASP	367	39.223	2.564	31.693	1.00	29.18
ATOM	1210	CA	ASP	367	38.594	3.233	30.560	1.00	32.72
ATOM	1211	CB	ASP	367	37.428	2.395	30.018	1.00	38.04
ATOM	1212	CG	ASP	367	37.855	0.995	29.606	1.00	42.43
ATOM	1213	OD1	ASP	367	38.913	0.852	28.956	1.00	35.95
ATOM	1214	OD2	ASP	367	37.115	0.034	29.917	1.00	51.42
ATOM	1215	C	ASP	367	38.093	4.631	30.881	1.00	33.71
ATOM	1216	O	ASP	367	38.059	5.506	30.013	1.00	38.30
ATOM	1217	N	THR	368	37.705	4.852	32.132	1.00	31.06
ATOM	1218	CA	THR	368	37.199	6.155	32.543	1.00	26.28
ATOM	1219	CB	THR	368	36.537	6.066	33.922	1.00	27.30
ATOM	1220	OG1	THR	368	35.461	5.127	33.861	1.00	33.42
ATOM	1221	CG2	THR	368	36.003	7.423	34.355	1.00	25.16
ATOM	1222	C	THR	368	38.303	7.194	32.593	1.00	21.13
ATOM	1223	O	THR	368	38.133	8.314	32.104	1.00	23.17
ATOM	1224	N	GLU	369	39.431	6.816	33.179	1.00	21.32
ATOM	1225	CA	GLU	369	40.565	7.720	33.317	1.00	28.00
ATOM	1226	CB	GLU	369	4				



ATOM	1227	CG	GLU	369	40.944	6.804	35.619	1.00	36.29
ATOM	1228	CD	GLU	369	41.834	6.026	36.546	1.00	41.03
ATOM	1229	OE1	GLU	369	42.361	4.967	36.123	1.00	42.05
ATOM	1230	OE2	GLU	369	41.986	6.458	37.705	1.00	42.03
ATOM	1231	C	GLU	369	41.201	8.047	31.970	1.00	25.57
ATOM	1232	O	GLU	369	41.626	9.175	31.741	1.00	20.56
ATOM	1233	N	VAL	370	41.249	7.055	31.080	1.00	25.39
ATOM	1234	CA	VAL	370	41.794	7.278	29.745	1.00	25.99
ATOM	1235	CB	VAL	370	42.005	5.936	28.977	1.00	26.15
ATOM	1236	CG1	VAL	370	42.450	6.216	27.539	1.00	27.65
ATOM	1237	CG2	VAL	370	43.056	5.086	29.685	1.00	17.70
ATOM	1238	C	VAL	370	40.814	8.164	28.966	1.00	26.49
ATOM	1239	O	VAL	370	41.226	9.038	28.202	1.00	28.16
ATOM	1240	N	ALA	371	39.514	7.950	29.184	1.00	21.01
ATOM	1241	CA	ALA	371	38.486	8.730	28.510	1.00	19.57
ATOM	1242	CB	ALA	371	37.116	8.136	28.783	1.00	18.62
ATOM	1243	C	ALA	371	38.512	10.191	28.947	1.00	23.48
ATOM	1244	O	ALA	371	38.500	11.103	28.111	1.00	32.67
ATOM	1245	N	LEU	372	38.540	10.414	30.256	1.00	22.89
ATOM	1246	CA	LEU	372	38.560	11.772	30.806	1.00	23.28
ATOM	1247	CB	LEU	372	38.517	11.709	32.343	1.00	27.76
ATOM	1248	CG	LEU	372	37.155	11.306	32.924	1.00	21.18
ATOM	1249	CD1	LEU	372	37.289	10.891	34.381	1.00	27.64
ATOM	1250	CD2	LEU	372	36.197	12.480	32.763	1.00	20.90
ATOM	1251	C	LEU	372	39.804	12.505	30.357	1.00	21.34
ATOM	1252	O	LEU	372	39.779	13.708	30.086	1.00	23.16
ATOM	1253	N	LEU	373	40.896	11.761	30.276	1.00	24.42
ATOM	1254	CA	LEU	373	42.177	12.302	29.855	1.00	23.78
ATOM	1255	CB	LEU	373	43.222	11.205	30.007	1.00	22.18
ATOM	1256	CG	LEU	373	44.724	11.456	30.036	1.00	31.52
ATOM	1257	CD1	LEU	373	45.099	12.565	31.001	1.00	31.93
ATOM	1258	CD2	LEU	373	45.382	10.152	30.460	1.00	30.24
ATOM	1259	C	LEU	373	42.025	12.757	28.399	1.00	25.69
ATOM	1260	O	LEU	373	42.469	13.842	28.025	1.00	30.13
ATOM	1261	N	GLN	374	41.370	11.934	27.587	1.00	26.24
ATOM	1262	CA	GLN	374	41.151	12.269	26.184	1.00	21.60
ATOM	1263	CB	GLN	374	40.501	11.091	25.444	1.00	24.57
ATOM	1264	CG	GLN	374	41.428	9.900	25.234	1.00	21.02
ATOM	1265	CD	GLN	374	40.762	8.744	24.501	1.00	22.86
ATOM	1266	OE1	GLN	374	41.407	7.754	24.174	1.00	24.07
ATOM	1267	NE2	GLN	374	39.466	8.865	24.249	1.00	25.59
ATOM	1268	C	GLN	374	40.267	13.498	26.070	1.00	20.66
ATOM	1269	O	GLN	374	40.518	14.366	25.242	1.00	24.47
ATOM	1270	N	ALA	375	39.237	13.579	26.902	1.00	16.26
ATOM	1271	CA	ALA	375	38.337	14.727	26.870	1.00	17.16</



ATOM	1273	C	ALA	375	39.056	16.024	27.252	1.00	25.13
ATOM	1274	O	ALA	375	38.722	17.100	26.750	1.00	23.81
ATOM	1275	N	VAL	376	40.036	15.926	28.156	1.00	24.57
ATOM	1276	CA	VAL	376	40.796	17.101	28.568	1.00	25.80
ATOM	1277	CB	VAL	376	41.711	16.792	29.814	1.00	26.48
ATOM	1278	CG1	VAL	376	42.625	17.971	30.102	1.00	23.20
ATOM	1279	CG2	VAL	376	40.845	16.521	31.044	1.00	19.08
ATOM	1280	C	VAL	376	41.653	17.580	27.396	1.00	25.69
ATOM	1281	O	VAL	376	41.775	18.780	27.151	1.00	27.87
ATOM	1282	N	LEU	377	42.249	16.637	26.666	1.00	23.09
ATOM	1283	CA	LEU	377	43.071	16.982	25.513	1.00	22.86
ATOM	1284	CB	LEU	377	43.748	15.730	24.962	1.00	18.50
ATOM	1285	CG	LEU	377	44.814	15.096	25.867	1.00	22.65
ATOM	1286	CD1	LEU	377	45.144	13.708	25.374	1.00	16.70
ATOM	1287	CD2	LEU	377	46.070	15.987	25.901	1.00	19.58
ATOM	1288	C	LEU	377	42.197	17.634	24.430	1.00	26.14
ATOM	1289	O	LEU	377	42.579	18.638	23.830	1.00	20.62
ATOM	1290	N	LEU	378	41.016	17.057	24.208	1.00	28.99
ATOM	1291	CA	LEU	378	40.076	17.578	23.218	1.00	28.87
ATOM	1292	CB	LEU	378	38.814	16.710	23.182	1.00	26.89
ATOM	1293	CG	LEU	378	37.637	17.167	22.311	1.00	28.83
ATOM	1294	CD1	LEU	378	38.053	17.273	20.840	1.00	27.97
ATOM	1295	CD2	LEU	378	36.496	16.175	22.478	1.00	27.69
ATOM	1296	C	LEU	378	39.693	19.025	23.504	1.00	31.09
ATOM	1297	O	LEU	378	39.812	19.883	22.629	1.00	31.77
ATOM	1298	N	MET	379	39.247	19.297	24.729	1.00	31.44
ATOM	1299	CA	MET	379	38.841	20.649	25.104	1.00	32.62
ATOM	1300	CB	MET	379	37.876	20.603	26.293	1.00	31.45
ATOM	1301	CG	MET	379	36.586	19.855	26.010	1.00	38.75
ATOM	1302	SD	MET	379	35.646	20.541	24.601	1.00	41.27
ATOM	1303	CE	MET	379	34.231	19.443	24.609	1.00	35.68
ATOM	1304	C	MET	379	39.980	21.613	25.421	1.00	33.72
ATOM	1305	O	MET	379	39.940	22.297	26.446	1.00	36.29
ATOM	1306	N	SER	380	40.981	21.676	24.543	1.00	34.49
ATOM	1307	CA	SER	380	42.116	22.585	24.721	1.00	33.97
ATOM	1308	CB	SER	380	43.371	22.025	24.061	1.00	31.24
ATOM	1309	OG	SER	380	43.771	20.814	24.674	1.00	39.42
ATOM	1310	C	SER	380	41.772	23.926	24.088	1.00	39.69
ATOM	1311	O	SER	380	41.787	24.069	22.864	1.00	44.64
ATOM	1312	N	SER	381	41.472	24.907	24.927	1.00	41.04
ATOM	1313	CA	SER	381	41.090	26.234	24.462	1.00	44.91
ATOM	1314	CB	SER	381	40.406	27.004	25.594	1.00	44.50
ATOM	1315	OG	SER	381	41.294	27.177	26.678	1.00	45.42
ATOM	1316	C	SER	381	42.231	27.084	23.921	1.00	44.59
ATOM	1317	O	SER	381	42.012	28.227	23.516	1.00	49.32

ATOM	1319	CA	ASP	382	44.571	27.315	23.407	1.00	43.93
ATOM	1320	CB	ASP	382	45.817	27.047	24.257	1.00	48.39
ATOM	1321	CG	ASP	382	46.319	25.632	24.113	1.00	53.23
ATOM	1322	OD1	ASP	382	45.590	24.702	24.517	1.00	56.97
ATOM	1323	OD2	ASP	382	47.440	25.449	23.584	1.00	58.91
ATOM	1324	C-	ASP	382	44.900	27.026	21.955	1.00	41.09
ATOM	1325	O	ASP	382	45.912	27.502	21.446	1.00	40.93
ATOM	1326	N	ARG	383	44.068	26.236	21.287	1.00	42.63
ATOM	1327	CA	ARG	383	44.316	25.937	19.876	1.00	43.32
ATOM	1328	CB	ARG	383	43.289	24.935	19.331	1.00	42.31
ATOM	1329	CG	ARG	383	43.174	23.619	20.095	1.00	40.83
ATOM	1330	CD	ARG	383	44.478	22.835	20.139	1.00	38.09
ATOM	1331	NE	ARG	383	44.271	21.542	20.787	1.00	37.33
ATOM	1332	CZ	ARG	383	45.235	20.690	21.115	1.00	38.35
ATOM	1333	NH1	ARG	383	46.505	20.972	20.850	1.00	33.70
ATOM	1334	NH2	ARG	383	44.922	19.545	21.704	1.00	35.46
ATOM	1335	C	ARG	383	44.166	27.256	19.127	1.00	44.96
ATOM	1336	O	ARG	383	43.214	28.006	19.361	1.00	45.60
ATOM	1337	N	PRO	384	45.112	27.574	18.230	1.00	45.33
ATOM	1338	CD	PRO	384	46.330	26.852	17.836	1.00	46.85
ATOM	1339	CA	PRO	384	45.024	28.830	17.484	1.00	47.37
ATOM	1340	CB	PRO	384	46.323	28.823	16.672	1.00	46.90
ATOM	1341	CG	PRO	384	47.257	27.998	17.552	1.00	46.41
ATOM	1342	C	PRO	384	43.788	28.910	16.590	1.00	48.29
ATOM	1343	O	PRO	384	43.394	27.927	15.960	1.00	48.34
ATOM	1344	N	GLY	385	43.176	30.090	16.552	1.00	49.88
ATOM	1345	CA	GLY	385	42.013	30.290	15.712	1.00	50.35
ATOM	1346	C	GLY	385	40.669	29.958	16.324	1.00	50.70
ATOM	1347	O	GLY	385	39.639	30.201	15.697	1.00	53.48
ATOM	1348	N	LEU	386	40.663	29.404	17.529	1.00	49.04
ATOM	1349	CA	LEU	386	39.405	29.057	18.182	1.00	50.53
ATOM	1350	CB	LEU	386	39.655	28.433	19.558	1.00	45.17
ATOM	1351	CG	LEU	386	40.245	27.019	19.544	1.00	48.26
ATOM	1352	CD1	LEU	386	40.502	26.564	20.970	1.00	41.68
ATOM	1353	CD2	LEU	386	39.285	26.065	18.836	1.00	38.40
ATOM	1354	C	LEU	386	38.495	30.268	18.319	1.00	52.13
ATOM	1355	O	LEU	386	38.955	31.395	18.476	1.00	53.67
ATOM	1356	N	ALA	387	37.193	30.020	18.261	1.00	53.42
ATOM	1357	CA	ALA	387	36.225	31.093	18.354	1.00	56.01
ATOM	1358	CB	ALA	387	35.221	30.976	17.202	1.00	56.47
ATOM	1359	C	ALA	387	35.482	31.144	19.681	1.00	55.52
ATOM	1360	O	ALA	387	35.491	32.171	20.358	1.00	53.75
ATOM	1361	N	CYS	388	34.854	30.038	20.065	1.00	56.03
ATOM	1362	CA	CYS	388	34.072	30.036	21.312	1.00	59.57
ATOM	1363	CB	CYS	388	32.724	29.351	21.089	1.00	59.23

ATOM	1365	C	CYS	388	34.846	29.289	22.398	1.00	62.18
ATOM	1366	O	CYS	388	34.458	28.190	22.790	1.00	67.88
ATOM	1367	N	VAL	389	35.955	29.950	22.760	1.00	60.78
ATOM	1368	CA	VAL	389	37.005	29.583	23.713	1.00	57.70
ATOM	1369	CB	VAL	389	38.202	30.580	23.565	1.00	57.09
ATOM	1370	CG1	VAL	389	39.351	30.194	24.494	1.00	59.03
ATOM	1371	CG2	VAL	389	38.671	30.618	22.124	1.00	53.98
ATOM	1372	C	VAL	389	36.661	29.515	25.195	1.00	57.77
ATOM	1373	O	VAL	389	36.943	28.513	25.851	1.00	60.94
ATOM	1374	N	GLU	390	36.102	30.594	25.732	1.00	52.68
ATOM	1375	CA	GLU	390	35.738	30.636	27.138	1.00	48.41
ATOM	1376	CB	GLU	390	35.001	31.928	27.451	1.00	45.19
ATOM	1377	C	GLU	390	34.868	29.439	27.459	1.00	47.63
ATOM	1378	O	GLU	390	34.986	28.837	28.529	1.00	51.95
ATOM	1379	N	ARG	391	34.002	29.082	26.517	1.00	47.11
ATOM	1380	CA	ARG	391	33.099	27.950	26.699	1.00	51.64
ATOM	1381	CB	ARG	391	32.050	27.930	25.588	1.00	54.22
ATOM	1382	CG	ARG	391	30.830	27.094	25.915	1.00	64.20
ATOM	1383	CD	ARG	391	29.867	27.074	24.748	1.00	73.80
ATOM	1384	NE	ARG	391	28.533	26.622	25.128	1.00	79.76
ATOM	1385	CZ	ARG	391	27.714	27.298	25.929	1.00	84.27
ATOM	1386	NH1	ARG	391	28.090	28.465	26.439	1.00	85.28
ATOM	1387	NH2	ARG	391	26.515	26.809	26.217	1.00	86.84
ATOM	1388	C	ARG	391	33.890	26.644	26.684	1.00	48.18
ATOM	1389	O	ARG	391	33.504	25.671	27.330	1.00	49.57
ATOM	1390	N	ILE	392	34.987	26.625	25.936	1.00	45.01
ATOM	1391	CA	ILE	392	35.835	25.440	25.858	1.00	48.77
ATOM	1392	CB	ILE	392	36.854	25.565	24.692	1.00	46.45
ATOM	1393	CG2	ILE	392	37.798	24.370	24.679	1.00	42.35
ATOM	1394	CG1	ILE	392	36.086	25.664	23.367	1.00	49.69
ATOM	1395	CD1	ILE	392	36.950	25.897	22.136	1.00	51.09
ATOM	1396	C	ILE	392	36.570	25.246	27.192	1.00	50.90
ATOM	1397	O	ILE	392	36.731	24.118	27.657	1.00	52.21
ATOM	1398	N	GLU	393	36.999	26.346	27.811	1.00	50.43
ATOM	1399	CA	GLU	393	37.673	26.267	29.101	1.00	50.30
ATOM	1400	CB	GLU	393	38.202	27.638	29.531	1.00	53.97
ATOM	1401	CG	GLU	393	39.322	28.168	28.658	1.00	62.18
ATOM	1402	CD	GLU	393	39.911	29.478	29.168	1.00	67.69
ATOM	1403	OE1	GLU	393	40.869	29.977	28.537	1.00	66.42
ATOM	1404	OE2	GLU	393	39.423	30.009	30.191	1.00	70.64
ATOM	1405	C	GLU	393	36.686	25.765	30.145	1.00	49.31
ATOM	1406	O	GLU	393	37.018	24.923	30.980	1.00	49.53
ATOM	1407	N	LYS	394	35.468	26.286	30.090	1.00	46.07
ATOM	1408	CA	LYS	394	34.428	25.893	31.022	1.00	45.76
ATOM	1409	CB	LYS	394	33.147	26.666	30.727	1.00	4

ATOM	1411	O	LYS	394	33.982	23.699	31.911	1.00	49.13
ATOM	1412	N	TYR	395	34.223	23.887	29.679	1.00	46.57
ATOM	1413	CA	TYR	395	34.014	22.467	29.427	1.00	43.33
ATOM	1414	CB	TYR	395	33.818	22.211	27.929	1.00	48.44
ATOM	1415	CG	TYR	395	32.493	22.710	27.335	1.00	53.83
ATOM	1416	CD1	TYR	395	32.302	22.727	25.947	1.00	56.43
ATOM	1417	CE1	TYR	395	31.078	23.148	25.374	1.00	59.73
ATOM	1418	CD2	TYR	395	31.434	23.132	28.153	1.00	56.47
ATOM	1419	CE2	TYR	395	30.198	23.559	27.592	1.00	62.60
ATOM	1420	CZ	TYR	395	30.037	23.562	26.200	1.00	63.18
ATOM	1421	OH	TYR	395	28.834	23.962	25.635	1.00	64.46
ATOM	1422	C	TYR	395	35.189	21.635	29.938	1.00	37.30
ATOM	1423	O	TYR	395	34.993	20.599	30.564	1.00	34.10
ATOM	1424	N	GLN	396	36.408	22.091	29.671	1.00	31.92
ATOM	1425	CA	GLN	396	37.584	21.363	30.120	1.00	34.81
ATOM	1426	CB	GLN	396	38.861	21.987	29.560	1.00	32.64
ATOM	1427	CG	GLN	396	40.114	21.183	29.882	1.00	29.57
ATOM	1428	CD	GLN	396	41.370	21.827	29.352	1.00	29.46
ATOM	1429	OE1	GLN	396	41.648	22.982	29.649	1.00	34.65
ATOM	1430	NE2	GLN	396	42.139	21.088	28.570	1.00	27.21
ATOM	1431	C	GLN	396	37.647	21.342	31.647	1.00	37.13
ATOM	1432	O	GLN	396	37.939	20.302	32.236	1.00	37.36
ATOM	1433	N	ASP	397	37.371	22.484	32.284	1.00	38.61
ATOM	1434	CA	ASP	397	37.393	22.555	33.742	1.00	40.37
ATOM	1435	CB	ASP	397	37.099	23.973	34.240	1.00	40.51
ATOM	1436	CG	ASP	397	38.130	24.974	33.772	1.00	43.77
ATOM	1437	OD1	ASP	397	39.330	24.632	33.775	1.00	46.50
ATOM	1438	OD2	ASP	397	37.750	26.109	33.422	1.00	51.34
ATOM	1439	C	ASP	397	36.352	21.601	34.295	1.00	38.62
ATOM	1440	O	ASP	397	36.515	21.034	35.372	1.00	39.20
ATOM	1441	N	SER	398	35.282	21.423	33.540	1.00	37.84
ATOM	1442	CA	SER	398	34.221	20.524	33.942	1.00	37.80
ATOM	1443	CB	SER	398	33.039	20.669	32.984	1.00	34.28
ATOM	1444	OG	SER	398	31.981	19.815	33.360	1.00	46.60
ATOM	1445	C	SER	398	34.752	19.082	33.939	1.00	38.41
ATOM	1446	O	SER	398	34.372	18.274	34.787	1.00	39.98
ATOM	1447	N	PHE	399	35.630	18.772	32.987	1.00	34.82
ATOM	1448	CA	PHE	399	36.213	17.433	32.885	1.00	35.96
ATOM	1449	CB	PHE	399	36.809	17.181	31.493	1.00	35.75
ATOM	1450	CG	PHE	399	35.775	16.936	30.419	1.00	39.30
ATOM	1451	CD1	PHE	399	35.640	17.826	29.344	1.00	39.86
ATOM	1452	CD2	PHE	399	34.936	15.819	30.487	1.00	36.81
ATOM	1453	CE1	PHE	399	34.674	17.607	28.330	1.00	41.25
ATOM	1454	CE2	PHE	399	33.962	15.577	29.488	1.00	43.61
ATOM	1455	CZ	PHE	399	33.829	16.480	28.402		



ATOM	1457	O	PHE	399	37.406	16.139	34.512	1.00	26.86
ATOM	1458	N	LEU	400	38.132	18.239	34.118	1.00	31.47
ATOM	1459	CA	LEU	400	39.213	18.162	35.086	1.00	37.41
ATOM	1460	CB	LEU	400	40.051	19.441	35.038	1.00	34.24
ATOM	1461	CG	LEU	400	40.934	19.574	33.788	1.00	35.10
ATOM	1462	CD1	LEU	400	41.469	20.991	33.651	1.00	26.60
ATOM	1463	CD2	LEU	400	42.077	18.569	33.884	1.00	29.44
ATOM	1464	C	LEU	400	38.666	17.931	36.491	1.00	38.84
ATOM	1465	O	LEU	400	39.137	17.049	37.205	1.00	40.38
ATOM	1466	N	LEU	401	37.654	18.703	36.870	1.00	42.79
ATOM	1467	CA	LEU	401	37.056	18.584	38.197	1.00	43.48
ATOM	1468	CB	LEU	401	35.997	19.675	38.406	1.00	44.73
ATOM	1469	CG	LEU	401	35.322	19.737	39.779	1.00	51.39
ATOM	1470	CD1	LEU	401	36.359	20.002	40.866	1.00	50.11
ATOM	1471	CD2	LEU	401	34.273	20.834	39.778	1.00	49.30
ATOM	1472	C	LEU	401	36.433	17.215	38.409	1.00	41.62
ATOM	1473	O	LEU	401	36.563	16.622	39.482	1.00	45.14
ATOM	1474	N	ALA	402	35.744	16.712	37.389	1.00	37.92
ATOM	1475	CA	ALA	402	35.115	15.402	37.484	1.00	29.90
ATOM	1476	CB	ALA	402	34.196	15.187	36.297	1.00	30.70
ATOM	1477	C	ALA	402	36.203	14.336	37.508	1.00	28.88
ATOM	1478	O	ALA	402	36.083	13.322	38.188	1.00	32.14
ATOM	1479	N	PHE	403	37.274	14.588	36.764	1.00	31.07
ATOM	1480	CA	PHE	403	38.402	13.656	36.661	1.00	29.90
ATOM	1481	CB	PHE	403	39.396	14.178	35.605	1.00	27.03
ATOM	1482	CG	PHE	403	40.434	13.146	35.140	1.00	26.97
ATOM	1483	CD1	PHE	403	41.362	13.509	34.149	1.00	25.55
ATOM	1484	CD2	PHE	403	40.475	11.841	35.664	1.00	19.75
ATOM	1485	CE1	PHE	403	42.331	12.588	33.679	1.00	27.90
ATOM	1486	CE2	PHE	403	41.441	10.899	35.206	1.00	22.56
ATOM	1487	CZ	PHE	403	42.371	11.273	34.210	1.00	22.24
ATOM	1488	C	PHE	403	39.081	13.523	38.023	1.00	28.82
ATOM	1489	O	PHE	403	39.313	12.413	38.495	1.00	26.00
ATOM	1490	N	GLU	404	39.405	14.652	38.652	1.00	30.25
ATOM	1491	CA	GLU	404	40.039	14.627	39.966	1.00	34.03
ATOM	1492	CB	GLU	404	40.264	16.046	40.497	1.00	39.45
ATOM	1493	CG	GLU	404	40.987	16.076	41.839	1.00	47.68
ATOM	1494	CD	GLU	404	41.062	17.465	42.446	1.00	54.02
ATOM	1495	OE1	GLU	404	41.607	18.380	41.796	1.00	57.27
ATOM	1496	OE2	GLU	404	40.573	17.638	43.585	1.00	63.85
ATOM	1497	C	GLU	404	39.164	13.860	40.960	1.00	36.01
ATOM	1498	O	GLU	404	39.661	12.997	41.701	1.00	38.64
ATOM	1499	N	HIS	405	37.870	14.168	40.975	1.00	29.56
ATOM	1500	CA	HIS	405	36.949	13.508	41.892	1.00	31.69
ATOM	1501	CB	HIS	405	35.534	14.077	41.757		



ATOM	1503	CD2 HIS	405	36.308	16.361	42.730	1.00	34.58
ATOM	1504	ND1 HIS	405	34.207	16.187	42.146	1.00	32.43
ATOM	1505	CE1 HIS	405	34.385	17.414	42.598	1.00	36.15
ATOM	1506	NE2 HIS	405	35.650	17.549	42.960	1.00	39.84
ATOM	1507	C HIS	405	36.904	12.013	41.673	1.00	34.21
ATOM	1508	O HIS	405	36.700	11.247	42.624	1.00	37.06
ATOM	1509	N TYR	406	37.081	11.594	40.419	1.00	30.83
ATOM	1510	CA TYR	406	37.059	10.173	40.093	1.00	28.85
ATOM	1511	CB TYR	406	37.018	9.959	38.575	1.00	31.48
ATOM	1512	CG TYR	406	36.879	8.490	38.181	1.00	23.49
ATOM	1513	CD1 TYR	406	35.683	7.798	38.397	1.00	19.42
ATOM	1514	CE1 TYR	406	35.556	6.427	38.059	1.00	23.80
ATOM	1515	CD2 TYR	406	37.950	7.794	37.624	1.00	21.81
ATOM	1516	CE2 TYR	406	37.838	6.421	37.278	1.00	24.64
ATOM	1517	CZ TYR	406	36.639	5.753	37.503	1.00	21.56
ATOM	1518	OH TYR	406	36.537	4.404	37.186	1.00	24.96
ATOM	1519	C TYR	406	38.318	9.526	40.638	1.00	24.24
ATOM	1520	O TYR	406	38.308	8.375	41.050	1.00	27.08
ATOM	1521	N ILE	407	39.407	10.278	40.617	1.00	25.76
ATOM	1522	CA ILE	407	40.688	9.799	41.105	1.00	33.75
ATOM	1523	CB ILE	407	41.815	10.822	40.796	1.00	34.23
ATOM	1524	CG2 ILE	407	43.121	10.400	41.435	1.00	32.46
ATOM	1525	CG1 ILE	407	41.959	10.972	39.275	1.00	43.30
ATOM	1526	CD1 ILE	407	42.267	9.677	38.523	1.00	40.40
ATOM	1527	C ILE	407	40.620	9.556	42.613	1.00	39.03
ATOM	1528	O ILE	407	41.192	8.583	43.107	1.00	35.18
ATOM	1529	N ASN	408	39.916	10.440	43.335	1.00	37.25
ATOM	1530	CA ASN	408	39.778	10.292	44.777	1.00	37.01
ATOM	1531	CB ASN	408	39.099	11.514	45.400	1.00	32.27
ATOM	1532	CG ASN	408	39.887	12.790	45.187	1.00	33.56
ATOM	1533	OD1 ASN	408	41.118	12.785	45.225	1.00	31.99
ATOM	1534	ND2 ASN	408	39.182	13.903	44.996	1.00	31.23
ATOM	1535	C ASN	408	38.961	9.046	45.055	1.00	38.14
ATOM	1536	O ASN	408	39.303	8.243	45.920	1.00	42.16
ATOM	1537	N TYR	409	37.874	8.894	44.303	1.00	35.62
ATOM	1538	CA TYR	409	37.002	7.733	44.412	1.00	35.91
ATOM	1539	CB TYR	409	35.929	7.804	43.323	1.00	34.41
ATOM	1540	CG TYR	409	35.196	6.495	43.066	1.00	38.73
ATOM	1541	CD1 TYR	409	34.266	5.982	43.980	1.00	41.34
ATOM	1542	CE1 TYR	409	33.600	4.745	43.741	1.00	47.16
ATOM	1543	CD2 TYR	409	35.461	5.752	41.907	1.00	46.20
ATOM	1544	CE2 TYR	409	34.814	4.518	41.651	1.00	50.74
ATOM	1545	CZ TYR	409	33.891	4.023	42.573	1.00	50.88
ATOM	1546	OH TYR	409	33.262	2.816	42.302	1.00	53.14
ATOM	1547	C TYR	409	37.827	6.459	44.240	1.00	38.16
ATOM	1548	O TYR	409	37.806	5.561	45.082	1.00	41.83

ATOM	1549	N	ARG	410	38.551	6.399	43.125	1.00	42.25
ATOM	1550	CA	ARG	410	39.410	5.272	42.765	1.00	42.83
ATOM	1551	CB	ARG	410	40.029	5.540	41.392	1.00	36.83
ATOM	1552	CG	ARG	410	39.055	5.397	40.249	1.00	34.32
ATOM	1553	CD	ARG	410	39.134	3.996	39.681	1.00	36.62
ATOM	1554	NE	ARG	410	40.420	3.787	39.013	1.00	38.64
ATOM	1555	CZ	ARG	410	40.832	2.625	38.517	1.00	35.73
ATOM	1556	NH1	ARG	410	40.068	1.548	38.617	1.00	33.17
ATOM	1557	NH2	ARG	410	42.006	2.544	37.916	1.00	32.70
ATOM	1558	C	ARG	410	40.520	5.039	43.780	1.00	46.67
ATOM	1559	O	ARG	410	40.900	3.901	44.053	1.00	41.78
ATOM	1560	N	LYS	411	41.026	6.140	44.325	1.00	52.99
ATOM	1561	CA	LYS	411	42.109	6.141	45.298	1.00	58.32
ATOM	1562	CB	LYS	411	41.565	5.956	46.731	1.00	64.99
ATOM	1563	CG	LYS	411	40.660	4.763	46.977	1.00	70.48
ATOM	1564	CD	LYS	411	40.034	4.866	48.364	1.00	77.18
ATOM	1565	CE	LYS	411	39.053	3.732	48.625	1.00	84.30
ATOM	1566	NZ	LYS	411	38.392	3.865	49.958	1.00	86.48
ATOM	1567	C	LYS	411	43.238	5.163	45.000	1.00	56.66
ATOM	1568	O	LYS	411	43.329	4.075	45.575	1.00	55.47
ATOM	1569	N	HIS	412	44.091	5.582	44.070	1.00	54.67
ATOM	1570	CA	HIS	412	45.266	4.823	43.657	1.00	48.67
ATOM	1571	CB	HIS	412	45.878	5.442	42.393	1.00	43.14
ATOM	1572	CG	HIS	412	45.073	5.218	41.156	1.00	41.36
ATOM	1573	CD2	HIS	412	44.084	5.952	40.584	1.00	35.44
ATOM	1574	ND1	HIS	412	45.220	4.093	40.364	1.00	38.19
ATOM	1575	CE1	HIS	412	44.357	4.150	39.363	1.00	34.75
ATOM	1576	NE2	HIS	412	43.659	5.263	39.474	1.00	35.52
ATOM	1577	C	HIS	412	46.264	4.932	44.793	1.00	46.35
ATOM	1578	O	HIS	412	46.326	5.951	45.479	1.00	42.73
ATOM	1579	N	HIS	413	47.049	3.883	44.993	1.00	48.92
ATOM	1580	CA	HIS	413	48.040	3.903	46.052	1.00	53.15
ATOM	1581	CB	HIS	413	48.148	2.515	46.688	1.00	55.27
ATOM	1582	CG	HIS	413	46.843	2.015	47.238	1.00	58.77
ATOM	1583	CD2	HIS	413	46.138	0.892	46.977	1.00	61.65
ATOM	1584	ND1	HIS	413	46.108	2.726	48.161	1.00	60.31
ATOM	1585	CE1	HIS	413	45.003	2.061	48.445	1.00	63.01
ATOM	1586	NE2	HIS	413	44.993	0.942	47.743	1.00	62.93
ATOM	1587	C	HIS	413	49.359	4.364	45.456	1.00	53.19
ATOM	1588	O	HIS	413	50.335	3.617	45.390	1.00	54.93
ATOM	1589	N	VAL	414	49.343	5.612	44.999	1.00	53.77
ATOM	1590	CA	VAL	414	50.487	6.282	44.389	1.00	51.06
ATOM	1591	CB	VAL	414	50.374	6.305	42.838	1.00	51.49
ATOM	1592	CG1	VAL	414	51.603	6.958	42.231	1.00	45.22
ATOM	1593	CG2	VAL	414	50.210	4.891	42.304	1.00	52.67
ATOM	1594	C	VAL	414					

ATOM	1595	O	VAL	414	49.418	8.401	44.774	1.00	55.49
ATOM	1596	N	THR	415	51.547	8.190	45.467	1.00	56.28
ATOM	1597	CA	THR	415	51.610	9.550	45.986	1.00	57.83
ATOM	1598	CB	THR	415	52.874	9.756	46.858	1.00	59.64
ATOM	1599	OG1	THR	415	52.922	11.115	47.311	1.00	66.69
ATOM	1600	CG2	THR	415	54.137	9.436	46.067	1.00	59.42
ATOM	1601	C	THR	415	51.599	10.577	44.855	1.00	56.98
ATOM	1602	O	THR	415	52.176	10.345	43.789	1.00	55.70
ATOM	1603	N	HIS	416	50.936	11.707	45.093	1.00	57.44
ATOM	1604	CA	HIS	416	50.835	12.786	44.108	1.00	57.34
ATOM	1605	CB	HIS	416	52.207	13.425	43.875	1.00	61.35
ATOM	1606	CG	HIS	416	52.860	13.940	45.123	1.00	69.78
ATOM	1607	CD2	HIS	416	54.049	13.633	45.695	1.00	71.42
ATOM	1608	ND1	HIS	416	52.283	14.901	45.922	1.00	72.49
ATOM	1609	CE1	HIS	416	53.087	15.165	46.938	1.00	75.50
ATOM	1610	NE2	HIS	416	54.165	14.410	46.819	1.00	73.91
ATOM	1611	C	HIS	416	50.301	12.260	42.773	1.00	53.79
ATOM	1612	O	HIS	416	50.769	12.667	41.710	1.00	52.81
ATOM	1613	N	PHE	417	49.318	11.366	42.824	1.00	48.05
ATOM	1614	CA	PHE	417	48.769	10.784	41.610	1.00	47.99
ATOM	1615	CB	PHE	417	47.652	9.799	41.940	1.00	46.11
ATOM	1616	CG	PHE	417	47.314	8.868	40.791	1.00	44.27
ATOM	1617	CD1	PHE	417	48.155	7.796	40.481	1.00	41.79
ATOM	1618	CD2	PHE	417	46.179	9.091	40.003	1.00	40.23
ATOM	1619	CE1	PHE	417	47.872	6.936	39.386	1.00	44.30
ATOM	1620	CE2	PHE	417	45.874	8.248	38.907	1.00	36.80
ATOM	1621	CZ	PHE	417	46.725	7.167	38.595	1.00	40.69
ATOM	1622	C	PHE	417	48.227	11.824	40.625	1.00	46.69
ATOM	1623	O	PHE	417	48.551	11.787	39.436	1.00	43.35
ATOM	1624	N	TRP	418	47.410	12.746	41.124	1.00	45.14
ATOM	1625	CA	TRP	418	46.821	13.775	40.276	1.00	44.89
ATOM	1626	CB	TRP	418	45.808	14.604	41.077	1.00	42.24
ATOM	1627	CG	TRP	418	45.096	15.646	40.259	1.00	47.11
ATOM	1628	CD2	TRP	418	44.186	15.417	39.159	1.00	46.98
ATOM	1629	CE2	TRP	418	43.786	16.678	38.676	1.00	48.94
ATOM	1630	CE3	TRP	418	43.676	14.261	38.548	1.00	45.23
ATOM	1631	CD1	TRP	418	45.204	17.003	40.387	1.00	46.24
ATOM	1632	NE1	TRP	418	44.425	17.637	39.448	1.00	50.63
ATOM	1633	CZ2	TRP	418	42.891	16.839	37.598	1.00	45.46
ATOM	1634	CZ3	TRP	418	42.780	14.411	37.468	1.00	44.50
ATOM	1635	CH2	TRP	418	42.403	15.696	37.009	1.00	47.55
ATOM	1636	C	TRP	418	47.862	14.676	39.598	1.00	43.88
ATOM	1637	O	TRP	418	47.834	14.842	38.383	1.00	43.17
ATOM	1638	N	PRO	419	48.788	15.281	40.369	1.00	43.55
ATOM	1639	CD	PRO	419	49.006	15.290	41.826	1.00	41.

ATOM	1641	CB	PRO	419	50.626	16.627	40.912	1.00	39.21
ATOM	1642	CG	PRO	419	49.593	16.667	42.017	1.00	39.25
ATOM	1643	C	PRO	419	50.616	15.363	38.701	1.00	36.28
ATOM	1644	O	PRO	419	50.940	15.882	37.638	1.00	37.08
ATOM	1645	N	LYS	420	50.959	14.124	39.033	1.00	35.96
ATOM	1646	CA	LYS	420	51.742	13.281	38.132	1.00	40.82
ATOM	1647	CB	LYS	420	52.094	11.945	38.792	1.00	40.78
ATOM	1648	CG	LYS	420	53.086	12.046	39.933	1.00	48.62
ATOM	1649	CD	LYS	420	53.391	10.668	40.497	1.00	55.12
ATOM	1650	CE	LYS	420	54.395	10.741	41.635	1.00	53.26
ATOM	1651	NZ	LYS	420	54.719	9.388	42.152	1.00	52.69
ATOM	1652	C	LYS	420	50.957	13.005	36.860	1.00	40.29
ATOM	1653	O	LYS	420	51.516	12.989	35.764	1.00	39.66
ATOM	1654	N	LEU	421	49.658	12.786	37.023	1.00	38.33
ATOM	1655	CA	LEU	421	48.784	12.507	35.903	1.00	37.60
ATOM	1656	CB	LEU	421	47.417	12.074	36.428	1.00	43.66
ATOM	1657	CG	LEU	421	46.386	11.479	35.474	1.00	46.50
ATOM	1658	CD1	LEU	421	46.946	10.253	34.770	1.00	45.15
ATOM	1659	CD2	LEU	421	45.154	11.107	36.279	1.00	51.31
ATOM	1660	C	LEU	421	48.661	13.747	35.014	1.00	39.59
ATOM	1661	O	LEU	421	48.599	13.638	33.791	1.00	40.66
ATOM	1662	N	LEU	422	48.642	14.928	35.623	1.00	39.57
ATOM	1663	CA	LEU	422	48.545	16.170	34.867	1.00	38.63
ATOM	1664	CB	LEU	422	48.313	17.357	35.802	1.00	41.79
ATOM	1665	CG	LEU	422	46.996	17.407	36.581	1.00	42.74
ATOM	1666	CD1	LEU	422	47.010	18.606	37.515	1.00	42.89
ATOM	1667	CD2	LEU	422	45.823	17.494	35.628	1.00	39.27
ATOM	1668	C	LEU	422	49.808	16.410	34.039	1.00	40.47
ATOM	1669	O	LEU	422	49.747	17.029	32.979	1.00	47.83
ATOM	1670	N	MET	423	50.949	15.936	34.519	1.00	34.27
ATOM	1671	CA	MET	423	52.187	16.103	33.774	1.00	35.25
ATOM	1672	CB	MET	423	53.403	15.716	34.622	1.00	32.56
ATOM	1673	CG	MET	423	53.675	16.654	35.774	1.00	40.70
ATOM	1674	SD	MET	423	55.226	16.278	36.597	1.00	47.65
ATOM	1675	CE	MET	423	54.920	14.601	37.163	1.00	47.16
ATOM	1676	C	MET	423	52.164	15.254	32.502	1.00	35.13
ATOM	1677	O	MET	423	52.934	15.499	31.570	1.00	29.85
ATOM	1678	N	LYS	424	51.285	14.252	32.482	1.00	31.56
ATOM	1679	CA	LYS	424	51.152	13.384	31.316	1.00	32.29
ATOM	1680	CB	LYS	424	50.373	12.115	31.681	1.00	30.56
ATOM	1681	CG	LYS	424	51.106	11.178	32.631	1.00	30.07
ATOM	1682	CD	LYS	424	52.248	10.482	31.938	1.00	33.22
ATOM	1683	CE	LYS	424	53.059	9.593	32.875	1.00	28.75
ATOM	1684	NZ	LYS	424	53.868	10.383	33.833	1.00	31.01
ATOM	1685	C	LYS	424	50.435	14.150	30.197		



ATOM	1687	N	VAL	425	49.514	15.036	30.573	1.00	23.53
ATOM	1688	CA	VAL	425	48.792	15.849	29.601	1.00	28.91
ATOM	1689	CB	VAL	425	47.808	16.829	30.295	1.00	29.44
ATOM	1690	CG1	VAL	425	47.148	17.737	29.273	1.00	28.81
ATOM	1691	CG2	VAL	425	46.744	16.049	31.057	1.00	31.22
ATOM	1692	C	VAL	425	49.822	16.669	28.831	1.00	32.03
ATOM	1693	O	VAL	425	49.771	16.769	27.605	1.00	31.95
ATOM	1694	N	THR	426	50.763	17.247	29.570	1.00	33.61
ATOM	1695	CA	THR	426	51.821	18.057	28.995	1.00	30.76
ATOM	1696	CB	THR	426	52.678	18.695	30.105	1.00	32.34
ATOM	1697	OG1	THR	426	51.842	19.535	30.912	1.00	33.07
ATOM	1698	CG2	THR	426	53.812	19.533	29.514	1.00	25.40
ATOM	1699	C	THR	426	52.712	17.225	28.086	1.00	32.53
ATOM	1700	O	THR	426	53.113	17.686	27.014	1.00	35.19
ATOM	1701	N	ASP	427	53.022	16.003	28.507	1.00	28.83
ATOM	1702	CA	ASP	427	53.858	15.130	27.695	1.00	35.12
ATOM	1703	CB	ASP	427	54.273	13.880	28.476	1.00	39.14
ATOM	1704	CG	ASP	427	55.122	14.212	29.693	1.00	45.80
ATOM	1705	OD1	ASP	427	56.052	15.034	29.556	1.00	41.97
ATOM	1706	OD2	ASP	427	54.869	13.642	30.775	1.00	50.06
ATOM	1707	C	ASP	427	53.124	14.726	26.422	1.00	33.94
ATOM	1708	O	ASP	427	53.737	14.617	25.362	1.00	38.02
ATOM	1709	N	LEU	428	51.818	14.512	26.529	1.00	27.15
ATOM	1710	CA	LEU	428	51.013	14.148	25.373	1.00	29.99
ATOM	1711	CB	LEU	428	49.602	13.719	25.802	1.00	22.49
ATOM	1712	CG	LEU	428	49.541	12.285	26.359	1.00	25.54
ATOM	1713	CD1	LEU	428	48.210	12.021	27.037	1.00	20.60
ATOM	1714	CD2	LEU	428	49.785	11.303	25.224	1.00	17.24
ATOM	1715	C	LEU	428	50.947	15.305	24.381	1.00	28.94
ATOM	1716	O	LEU	428	50.941	15.088	23.174	1.00	31.26
ATOM	1717	N	ARG	429	50.910	16.531	24.887	1.00	27.64
ATOM	1718	CA	ARG	429	50.877	17.694	24.011	1.00	28.13
ATOM	1719	CB	ARG	429	50.584	18.969	24.800	1.00	29.59
ATOM	1720	CG	ARG	429	49.224	18.980	25.455	1.00	34.85
ATOM	1721	CD	ARG	429	48.951	20.314	26.118	1.00	47.18
ATOM	1722	NE	ARG	429	47.657	20.358	26.797	1.00	57.93
ATOM	1723	CZ	ARG	429	46.473	20.193	26.200	1.00	63.62
ATOM	1724	NH1	ARG	429	46.402	19.972	24.889	1.00	60.71
ATOM	1725	NH2	ARG	429	45.356	20.257	26.919	1.00	62.38
ATOM	1726	C	ARG	429	52.229	17.819	23.304	1.00	29.81
ATOM	1727	O	ARG	429	52.294	18.209	22.143	1.00	30.81
ATOM	1728	N	MET	430	53.305	17.482	24.008	1.00	29.64
ATOM	1729	CA	MET	430	54.639	17.545	23.422	1.00	34.72
ATOM	1730	CB	MET	430	55.716	17.323	24.485	1.00	34.97
ATOM	1731	CG	MET	430	55.864	18.480	25.451	1.00	45.34



ATOM	1733	CE	MET	430	57.598	19.639	23.589	1.00	55.56
ATOM	1734	C	MET	430	54.778	16.500	22.325	1.00	34.01
ATOM	1735	O	MET	430	55.440	16.733	21.318	1.00	37.29
ATOM	1736	N	ILE	431	54.161	15.340	22.533	1.00	29.99
ATOM	1737	CA	ILE	431	54.197	14.279	21.545	1.00	28.82
ATOM	1738	CB	ILE	431	53.523	12.984	22.095	1.00	27.39
ATOM	1739	CG2	ILE	431	53.260	11.989	20.956	1.00	23.87
ATOM	1740	CG1	ILE	431	54.414	12.386	23.201	1.00	25.56
ATOM	1741	CD1	ILE	431	53.850	11.155	23.896	1.00	17.29
ATOM	1742	C	ILE	431	53.450	14.785	20.301	1.00	29.49
ATOM	1743	O	ILE	431	53.908	14.603	19.174	1.00	24.19
ATOM	1744	N	GLY	432	52.311	15.435	20.524	1.00	25.25
ATOM	1745	CA	GLY	432	51.542	15.971	19.419	1.00	30.38
ATOM	1746	C	GLY	432	52.334	16.997	18.614	1.00	32.75
ATOM	1747	O	GLY	432	52.410	16.895	17.387	1.00	36.38
ATOM	1748	N	ALA	433	52.930	17.974	19.294	1.00	26.77
ATOM	1749	CA	ALA	433	53.711	19.012	18.625	1.00	26.48
ATOM	1750	CB	ALA	433	54.182	20.047	19.631	1.00	19.90
ATOM	1751	C	ALA	433	54.902	18.407	17.890	1.00	30.73
ATOM	1752	O	ALA	433	55.207	18.787	16.760	1.00	31.60
ATOM	1753	N	CYS	434	55.582	17.467	18.537	1.00	33.22
ATOM	1754	CA	CYS	434	56.728	16.801	17.914	1.00	34.34
ATOM	1755	CB	CYS	434	57.339	15.808	18.895	1.00	35.20
ATOM	1756	SG	CYS	434	59.191	15.745	18.798	1.00	54.48
ATOM	1757	C	CYS	434	56.313	16.052	16.636	1.00	34.09
ATOM	1758	O	CYS	434	57.095	15.937	15.679	1.00	34.89
ATOM	1759	N	HIS	435	55.088	15.545	16.642	1.00	34.30
ATOM	1760	CA	HIS	435	54.570	14.818	15.501	1.00	35.44
ATOM	1761	CB	HIS	435	53.296	14.061	15.886	1.00	31.76
ATOM	1762	CG	HIS	435	52.587	13.469	14.715	1.00	32.03
ATOM	1763	CD2	HIS	435	52.735	12.277	14.092	1.00	28.61
ATOM	1764	ND1	HIS	435	51.665	14.177	13.970	1.00	28.48
ATOM	1765	CE1	HIS	435	51.284	13.453	12.941	1.00	33.27
ATOM	1766	NE2	HIS	435	51.920	12.284	12.985	1.00	31.57
ATOM	1767	C	HIS	435	54.311	15.750	14.319	1.00	32.74
ATOM	1768	O	HIS	435	54.504	15.363	13.175	1.00	32.87
ATOM	1769	N	ALA	436	53.881	16.975	14.608	1.00	31.01
ATOM	1770	CA	ALA	436	53.628	17.966	13.571	1.00	29.91
ATOM	1771	CB	ALA	436	53.221	19.290	14.197	1.00	21.23
ATOM	1772	C	ALA	436	54.911	18.135	12.769	1.00	33.86
ATOM	1773	O	ALA	436	54.892	18.128	11.541	1.00	36.10
ATOM	1774	N	SER	437	56.030	18.266	13.483	1.00	35.19
ATOM	1775	CA	SER	437	57.344	18.426	12.871	1.00	33.03
ATOM	1776	CB	SER	437	58.389	18.720	13.941	1.00	35.31
ATOM	1777	OG	SER	437	59.681	18.782	13.373	1.00	44.99
ATOM									

ATOM	1779	O	SER	437	58.374	17.269	11.034	1.00	37.54
ATOM	1780	N	ARG	438	57.427	16.012	12.642	1.00	37.32
ATOM	1781	CA	ARG	438	57.762	14.754	11.992	1.00	39.30
ATOM	1782	CB	ARG	438	57.517	13.572	12.941	1.00	42.97
ATOM	1783	CG	ARG	438	58.542	13.436	14.059	1.00	41.72
ATOM	1784	CD	ARG	438	59.926	13.212	13.484	1.00	45.23
ATOM	1785	NE	ARG	438	59.961	12.050	12.601	1.00	45.66
ATOM	1786	CZ	ARG	438	60.935	11.804	11.731	1.00	49.71
ATOM	1787	NH1	ARG	438	61.961	12.641	11.627	1.00	50.91
ATOM	1788	NH2	ARG	438	60.885	10.727	10.960	1.00	46.86
ATOM	1789	C	ARG	438	56.939	14.565	10.725	1.00	42.37
ATOM	1790	O	ARG	438	57.311	13.794	9.841	1.00	40.58
ATOM	1791	N	PHE	439	55.816	15.269	10.645	1.00	42.25
ATOM	1792	CA	PHE	439	54.957	15.170	9.479	1.00	42.81
ATOM	1793	CB	PHE	439	53.593	15.790	9.771	1.00	42.18
ATOM	1794	CG	PHE	439	52.594	15.597	8.656	1.00	42.48
ATOM	1795	CD1	PHE	439	52.173	14.312	8.295	1.00	47.09
ATOM	1796	CD2	PHE	439	52.086	16.696	7.961	1.00	39.76
ATOM	1797	CE1	PHE	439	51.256	14.110	7.234	1.00	49.17
ATOM	1798	CE2	PHE	439	51.174	16.524	6.896	1.00	45.10
ATOM	1799	CZ	PHE	439	50.751	15.225	6.532	1.00	46.36
ATOM	1800	C	PHE	439	55.626	15.905	8.322	1.00	44.79
ATOM	1801	O	PHE	439	55.596	15.444	7.181	1.00	40.26
ATOM	1802	N	LEU	440	56.236	17.049	8.629	1.00	42.77
ATOM	1803	CA	LEU	440	56.927	17.839	7.621	1.00	42.96
ATOM	1804	CB	LEU	440	57.421	19.156	8.216	1.00	37.19
ATOM	1805	CG	LEU	440	56.348	20.117	8.725	1.00	36.97
ATOM	1806	CD1	LEU	440	57.020	21.338	9.321	1.00	33.65
ATOM	1807	CD2	LEU	440	55.411	20.519	7.572	1.00	35.42
ATOM	1808	C	LEU	440	58.106	17.063	7.053	1.00	45.47
ATOM	1809	O	LEU	440	58.421	17.191	5.876	1.00	52.48
ATOM	1810	N	HIS	441	58.760	16.266	7.890	1.00	49.15
ATOM	1811	CA	HIS	441	59.893	15.473	7.435	1.00	54.76
ATOM	1812	CB	HIS	441	60.723	14.964	8.624	1.00	56.68
ATOM	1813	CG	HIS	441	61.515	16.026	9.323	1.00	62.73
ATOM	1814	CD2	HIS	441	62.851	16.166	9.508	1.00	65.73
ATOM	1815	ND1	HIS	441	60.929	17.098	9.966	1.00	66.01
ATOM	1816	CE1	HIS	441	61.871	17.845	10.518	1.00	65.55
ATOM	1817	NE2	HIS	441	63.044	17.306	10.258	1.00	60.09
ATOM	1818	C	HIS	441	59.417	14.292	6.589	1.00	55.93
ATOM	1819	O	HIS	441	60.084	13.908	5.630	1.00	57.33
ATOM	1820	N	MET	442	58.271	13.716	6.948	1.00	57.81
ATOM	1821	CA	MET	442	57.712	12.585	6.203	1.00	59.11
ATOM	1822	CB	MET	442	56.562	11.924	6.978	1.00	55.93
ATOM	1823	CG	MET	442	56.961	11.246	8.276	1.00	58.52
ATOM	1824	SD							

ATOM	1825	CE	MET	442	54.430	11.779	9.350	1.00	52.61
ATOM	1826	C	MET	442	57.178	13.065	4.854	1.00	60.31
ATOM	1827	O	MET	442	57.279	12.369	3.846	1.00	58.18
ATOM	1828	N	LYS	443	56.608	14.266	4.863	1.00	61.45
ATOM	1829	CA	LYS	443	56.038	14.871	3.669	1.00	64.90
ATOM	1830	CB	LYS	443	55.434	16.232	4.035	1.00	64.40
ATOM	1831	CG	LYS	443	54.589	16.872	2.945	1.00	69.12
ATOM	1832	CD	LYS	443	54.064	18.250	3.363	1.00	71.14
ATOM	1833	CE	LYS	443	53.138	18.183	4.575	1.00	73.43
ATOM	1834	NZ	LYS	443	52.668	19.534	5.015	1.00	67.97
ATOM	1835	C	LYS	443	57.112	15.030	2.585	1.00	67.29
ATOM	1836	O	LYS	443	56.800	15.218	1.406	1.00	67.90
ATOM	1837	N	VAL	444	58.373	14.941	2.996	1.00	66.57
ATOM	1838	CA	VAL	444	59.501	15.064	2.078	1.00	64.76
ATOM	1839	CB	VAL	444	60.618	15.940	2.693	1.00	62.76
ATOM	1840	CG1	VAL	444	61.767	16.092	1.712	1.00	64.00
ATOM	1841	CG2	VAL	444	60.062	17.301	3.072	1.00	59.27
ATOM	1842	C	VAL	444	60.091	13.693	1.744	1.00	68.61
ATOM	1843	O	VAL	444	60.145	13.294	0.577	1.00	70.60
ATOM	1844	N	GLU	445	60.520	12.972	2.775	1.00	70.71
ATOM	1845	CA	GLU	445	61.129	11.653	2.609	1.00	71.45
ATOM	1846	CB	GLU	445	61.808	11.233	3.916	1.00	72.36
ATOM	1847	C	GLU	445	60.181	10.547	2.148	1.00	71.46
ATOM	1848	O	GLU	445	60.588	9.390	2.042	1.00	73.02
ATOM	1849	N	CYS	446	58.925	10.895	1.871	1.00	71.12
ATOM	1850	CA	CYS	446	57.945	9.901	1.419	1.00	70.83
ATOM	1851	CB	CYS	446	57.031	9.485	2.581	1.00	71.05
ATOM	1852	SG	CYS	446	57.845	8.593	3.925	1.00	72.83
ATOM	1853	C	CYS	446	57.081	10.390	0.261	1.00	71.91
ATOM	1854	O	CYS	446	56.776	11.582	0.155	1.00	72.06
ATOM	1855	N	PRO	447	56.673	9.470	-0.635	1.00	73.12
ATOM	1856	CD	PRO	447	56.967	8.026	-0.671	1.00	72.88
ATOM	1857	CA	PRO	447	55.837	9.825	-1.784	1.00	74.22
ATOM	1858	CB	PRO	447	55.717	8.500	-2.537	1.00	72.98
ATOM	1859	CG	PRO	447	57.015	7.790	-2.161	1.00	74.77
ATOM	1860	C	PRO	447	54.479	10.343	-1.330	1.00	75.94
ATOM	1861	O	PRO	447	53.754	9.652	-0.616	1.00	76.67
ATOM	1862	N	THR	448	54.145	11.558	-1.755	1.00	76.91
ATOM	1863	CA	THR	448	52.879	12.197	-1.403	1.00	78.24
ATOM	1864	CB	THR	448	52.647	13.459	-2.261	1.00	81.33
ATOM	1865	OG1	THR	448	52.552	13.087	-3.643	1.00	84.46
ATOM	1866	CG2	THR	448	53.802	14.444	-2.089	1.00	83.51
ATOM	1867	C	THR	448	51.676	11.270	-1.580	1.00	77.42
ATOM	1868	O	THR	448	50.662	11.413	-0.894	1.00	77.65
ATOM	1869	N	GLU	449	51.795	10.319	-2.502	1.00	76.29
ATOM	1870	CA	GLU	449	50.720	9.375			

ATOM	1871	CB	GLU	449	51.048	8.572	-4.043	1.00	74.62
ATOM	1872	C	GLU	449	50.445	8.421	-1.622	1.00	73.49
ATOM	1873	O	GLU	449	49.310	7.973	-1.442	1.00	70.24
ATOM	1874	N	LEU	450	51.477	8.113	-0.840	1.00	70.80
ATOM	1875	CA	LEU	450	51.327	7.194	0.285	1.00	68.82
ATOM	1876	CB	LEU	450	52.693	6.644	0.705	1.00	71.91
ATOM	1877	CG	LEU	450	53.428	5.795	-0.336	1.00	76.62
ATOM	1878	CD1	LEU	450	54.799	5.414	0.195	1.00	77.95
ATOM	1879	CD2	LEU	450	52.617	4.546	-0.662	1.00	76.46
ATOM	1880	C	LEU	450	50.636	7.818	1.492	1.00	66.22
ATOM	1881	O	LEU	450	50.501	7.181	2.540	1.00	66.01
ATOM	1882	N	PHE	451	50.189	9.060	1.342	1.00	61.96
ATOM	1883	CA	PHE	451	49.513	9.750	2.428	1.00	58.44
ATOM	1884	CB	PHE	451	50.006	11.204	2.528	1.00	61.34
ATOM	1885	CG	PHE	451	51.466	11.343	2.923	1.00	63.02
ATOM	1886	CD1	PHE	451	52.488	10.888	2.077	1.00	62.92
ATOM	1887	CD2	PHE	451	51.812	11.932	4.146	1.00	63.07
ATOM	1888	CE1	PHE	451	53.855	11.029	2.437	1.00	65.12
ATOM	1889	CE2	PHE	451	53.167	12.085	4.531	1.00	64.66
ATOM	1890	CZ	PHE	451	54.195	11.628	3.673	1.00	67.12
ATOM	1891	C	PHE	451	48.005	9.756	2.219	1.00	56.41
ATOM	1892	O	PHE	451	47.501	10.471	1.350	1.00	56.56
ATOM	1893	N	PRO	452	47.260	8.954	3.009	1.00	53.28
ATOM	1894	CD	PRO	452	47.678	8.027	4.076	1.00	50.46
ATOM	1895	CA	PRO	452	45.797	8.910	2.866	1.00	50.26
ATOM	1896	CB	PRO	452	45.388	7.976	4.000	1.00	49.19
ATOM	1897	CG	PRO	452	46.558	7.010	4.039	1.00	45.89
ATOM	1898	C	PRO	452	45.183	10.305	2.974	1.00	49.62
ATOM	1899	O	PRO	452	45.727	11.176	3.644	1.00	52.35
ATOM	1900	N	PRO	453	44.034	10.530	2.313	1.00	51.50
ATOM	1901	CD	PRO	453	43.257	9.585	1.494	1.00	49.66
ATOM	1902	CA	PRO	453	43.354	11.830	2.335	1.00	50.89
ATOM	1903	CB	PRO	453	42.101	11.559	1.506	1.00	51.49
ATOM	1904	CG	PRO	453	42.600	10.524	0.521	1.00	50.82
ATOM	1905	C	PRO	453	43.030	12.405	3.706	1.00	50.99
ATOM	1906	O	PRO	453	43.264	13.588	3.953	1.00	54.17
ATOM	1907	N	LEU	454	42.479	11.576	4.592	1.00	51.21
ATOM	1908	CA	LEU	454	42.112	12.034	5.936	1.00	47.17
ATOM	1909	CB	LEU	454	41.305	10.951	6.660	1.00	44.44
ATOM	1910	CG	LEU	454	40.748	11.283	8.050	1.00	41.33
ATOM	1911	CD1	LEU	454	39.838	12.504	7.978	1.00	35.93
ATOM	1912	CD2	LEU	454	39.986	10.072	8.587	1.00	34.79
ATOM	1913	C	LEU	454	43.363	12.380	6.733	1.00	42.25
ATOM	1914	O	LEU	454	43.387	13.357	7.475	1.00	40.82
ATOM	1915	N	PHE	455	44.399	11.567	6.565	1.00	39.29
ATOM	1916	CA	PHE	455	45.674	11.77			



ATOM	1917	CB	PHE	455	46.655	10.679	6.802	1.00	47.22
ATOM	1918	CG	PHE	455	48.045	10.800	7.407	1.00	56.97
ATOM	1919	CD1	PHE	455	48.220	10.990	8.785	1.00	57.23
ATOM	1920	CD2	PHE	455	49.180	10.645	6.597	1.00	59.40
ATOM	1921	CE1	PHE	455	49.522	11.030	9.362	1.00	56.58
ATOM	1922	CE2	PHE	455	50.487	10.682	7.149	1.00	61.80
ATOM	1923	CZ	PHE	455	50.656	10.870	8.541	1.00	59.94
ATOM	1924	C	PHE	455	46.203	13.161	6.892	1.00	45.12
ATOM	1925	O	PHE	455	46.558	13.944	7.779	1.00	39.95
ATOM	1926	N	LEU	456	46.236	13.471	5.592	1.00	43.92
ATOM	1927	CA	LEU	456	46.704	14.767	5.123	1.00	44.08
ATOM	1928	CB	LEU	456	46.748	14.795	3.593	1.00	50.20
ATOM	1929	CG	LEU	456	47.796	13.921	2.903	1.00	55.79
ATOM	1930	CD1	LEU	456	47.527	13.869	1.408	1.00	54.70
ATOM	1931	CD2	LEU	456	49.187	14.473	3.193	1.00	53.01
ATOM	1932	C	LEU	456	45.782	15.871	5.616	1.00	44.65
ATOM	1933	O	LEU	456	46.219	16.987	5.887	1.00	45.93
ATOM	1934	N	GLU	457	44.500	15.549	5.726	1.00	44.56
ATOM	1935	CA	GLU	457	43.498	16.504	6.175	1.00	46.37
ATOM	1936	CB	GLU	457	42.138	15.854	6.133	1.00	50.16
ATOM	1937	C	GLU	457	43.759	17.039	7.579	1.00	43.60
ATOM	1938	O	GLU	457	43.867	18.245	7.795	1.00	42.69
ATOM	1939	N	VAL	458	43.847	16.117	8.528	1.00	43.21
ATOM	1940	CA	VAL	458	44.064	16.446	9.930	1.00	44.98
ATOM	1941	CB	VAL	458	44.020	15.159	10.802	1.00	44.83
ATOM	1942	CG1	VAL	458	44.180	15.510	12.277	1.00	49.72
ATOM	1943	CG2	VAL	458	42.708	14.427	10.567	1.00	40.89
ATOM	1944	C	VAL	458	45.368	17.178	10.209	1.00	42.72
ATOM	1945	O	VAL	458	45.393	18.139	10.974	1.00	42.88
ATOM	1946	N	PHE	459	46.451	16.743	9.574	1.00	44.53
ATOM	1947	CA	PHE	459	47.741	17.366	9.823	1.00	48.18
ATOM	1948	CB	PHE	459	48.784	16.269	10.064	1.00	43.60
ATOM	1949	CG	PHE	459	48.374	15.276	11.133	1.00	40.79
ATOM	1950	CD1	PHE	459	47.835	14.032	10.783	1.00	41.01
ATOM	1951	CD2	PHE	459	48.471	15.613	12.492	1.00	39.48
ATOM	1952	CE1	PHE	459	47.387	13.118	11.776	1.00	40.62
ATOM	1953	CE2	PHE	459	48.032	14.715	13.506	1.00	36.87
ATOM	1954	CZ	PHE	459	47.489	13.463	13.146	1.00	36.39
ATOM	1955	C	PHE	459	48.234	18.348	8.763	1.00	52.71
ATOM	1956	O	PHE	459	49.336	18.878	8.877	1.00	51.34
ATOM	1957	N	GLU	460	47.397	18.594	7.752	1.00	59.56
ATOM	1958	CA	GLU	460	47.695	19.509	6.647	1.00	66.14
ATOM	1959	CB	GLU	460	47.818	20.944	7.158	1.00	67.76
ATOM	1960	CG	GLU	460	46.536	21.511	7.724	1.00	78.99
ATOM	1961	CD	GLU	460	46.680	22.965	8.116	1.00	86.08
ATOM	1962								



ATOM	1963	OE2	GLU	460	46.460	23.289	9.301	1.00	91.63	
ATOM	1964	C	GLU	460	48.940	19.163	5.836	1.00	69.17	
ATOM	1965	O	GLU	460	48.784	18.759	4.660	1.00	69.49	
ATOM	1966	OXT	GLU	460	50.057	19.298	6.379	1.00	76.70	
ATOM	1967	C1	TRI	1	47.283	4.313	16.972	1.00	44.70	
ATOM	1968	C2	TRI	1	51.052	6.807	13.814	1.00	34.01	
ATOM	1969	C3	TRI	1	47.289	4.043	15.500	1.00	37.90	
ATOM	1970	C4	TRI	1	51.936	6.615	12.728	1.00	33.38	
ATOM	1971	C5	TRI	1	48.462	4.501	14.746	1.00	46.53	
ATOM	1972	C6	TRI	1	52.294	7.653	11.847	1.00	42.90	
ATOM	1973	C7	TRI	1	49.577	5.179	15.334	1.00	34.63	
ATOM	1974	C8	TRI	1	51.717	9.015	12.071	1.00	38.34	
ATOM	1975	C9	TRI	1	49.492	5.383	16.723	1.00	43.89	
ATOM	1976	C10	TRI	1	50.779	9.237	13.172	1.00	40.43	
ATOM	1977	C11	TRI	1	48.354	4.960	17.533	1.00	41.82	
ATOM	1978	C12	TRI	1	50.449	8.116	14.055	1.00	35.64	
ATOM	1979	C13	TRI	1	46.287	3.725	17.959	1.00	36.78	
ATOM	1980	C15	TRI	1	44.825	4.150	17.865	1.00	40.69	
ATOM	1981	I1	TRI	1	48.684	4.002	12.609	1.00	40.26	
ATOM	1982	I2	TRI	1	53.597	7.174	10.336	1.00	46.70	
ATOM	1983	I3	TRI	1	51.362	6.218	17.644	1.00	36.54	
ATOM	1984	O3	TRI	1	44.546	5.255	17.329	1.00	54.78	
ATOM	1985	O2	TRI	1	50.831	5.617	14.667	1.00	28.44	
ATOM	1986	O1	TRI	1	52.207	10.160	11.342	1.00	43.65	
ATOM	1987	O4	TRI	1	44.021	3.333	18.352	1.00	42.95	
ATOM	1	AS	CAC	501	60.548	16.977	16.916	1.00	65.97	AS
ATOM	2	AS	CAC	502	27.863	16.627	16.796	1.00	89.34	AS
ATOM	3	AS	CAC	503	29.889	28.698	21.811	1.00	100.00	AS
ATOM	4	AS	CAC	504	33.547	24.203	8.880	1.00	100.00	AS
ATOM	5	O	HOH	505	42.365	8.872	4.597	1.00	53.88	HOH
ATOM	6	O	HOH	506	33.545	30.973	24.585	1.00	40.33	HOH
ATOM	7	O	HOH	507	37.040	1.824	12.671	1.00	61.87	HOH
ATOM	8	O	HOH	508	44.105	4.635	6.023	1.00	40.68	HOH
ATOM	9	O	HOH	509	52.686	13.817	-6.263	1.00	54.00	HOH
ATOM	10	O	HOH	510	50.186	12.691	-5.997	1.00	55.36	HOH
ATOM	11	O	HOH	511	49.278	18.540	14.006	1.00	34.79	HOH
ATOM	12	O	HOH	512	25.541	28.885	21.206	1.00	55.42	HOH
ATOM	13	O	HOH	513	27.346	31.063	27.398	1.00	58.30	HOH
ATOM	14	O	HOH	514	40.790	19.192	39.234	1.00	50.35	HOH
ATOM	15	O	HOH	515	37.467	0.637	37.293	1.00	37.46	HOH
ATOM	16	O	HOH	516	36.155	3.879	47.189	1.00	61.37	HOH
ATOM	17	O	HOH	517	35.410	5.865	50.995	1.00	63.46	HOH
ATOM	18	O	HOH	518	33.622	5.440	47.570	1.00	53.87	HOH
ATOM	19	O	HOH	519	64.787	6.888	11.882	1.00	51.15	HOH
ATOM	20	O	HOH	520	61.109	-8.688	27.722	1.00	61.70	HOH
ATOM	21	O	HOH	521	49.869	-5.472	30.343	1.00	40.50	HOH



## ABSTRACT OF THE DISCLOSURE

The present invention provides new methods, particularly computational methods, and compositions for the generation of nuclear receptor synthetic ligands based on the three dimensional structure of nuclear receptors, particularly the thyroid receptor (herein referred to as "TR"). Also provided are crystals, nuclear receptor synthetic ligands, and related methods.

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Attorney Docket No: UCAL-246/02/1US  
96-026-5

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Date:

10 August 2000

By:



Vladimir Skliba

## IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In re application of BAXTER, John D. et al.

Serial No.: Not yet assigned

Examiner: Not yet assigned

Filed: August 10, 2000

Art Unit: Not yet assigned

For: NUCLEAR RECEPTOR LIGANDS AND LIGAND BINDING DOMAINS

BOX PATENT APPLICATION  
Assistant Commissioner for Patents  
Washington, D.C. 20231

### LETTER TO OFFICIAL DRAFTSPERSON

Enclosed are the formal drawings to replace the informal drawings originally filed in this application. The specification consists of 50 sheets of drawings, i.e. 12 sheets of black and white photographs, 34 sheets of black and white drawings, and 4 sheets of color photographs. The color photographs have been submitted in triplicate. Attached hereto are the following:

1. 12 sheets of black and white photographs;
2. 3 sets of the four color photographs, i.e. 12 sheets of color photographs;
3. 34 sheets of black and white drawings;

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MCJ:AKR:hh

By:

Madison C. Jellins  
Reg. No. 35,555

[illegible]



FIG.1

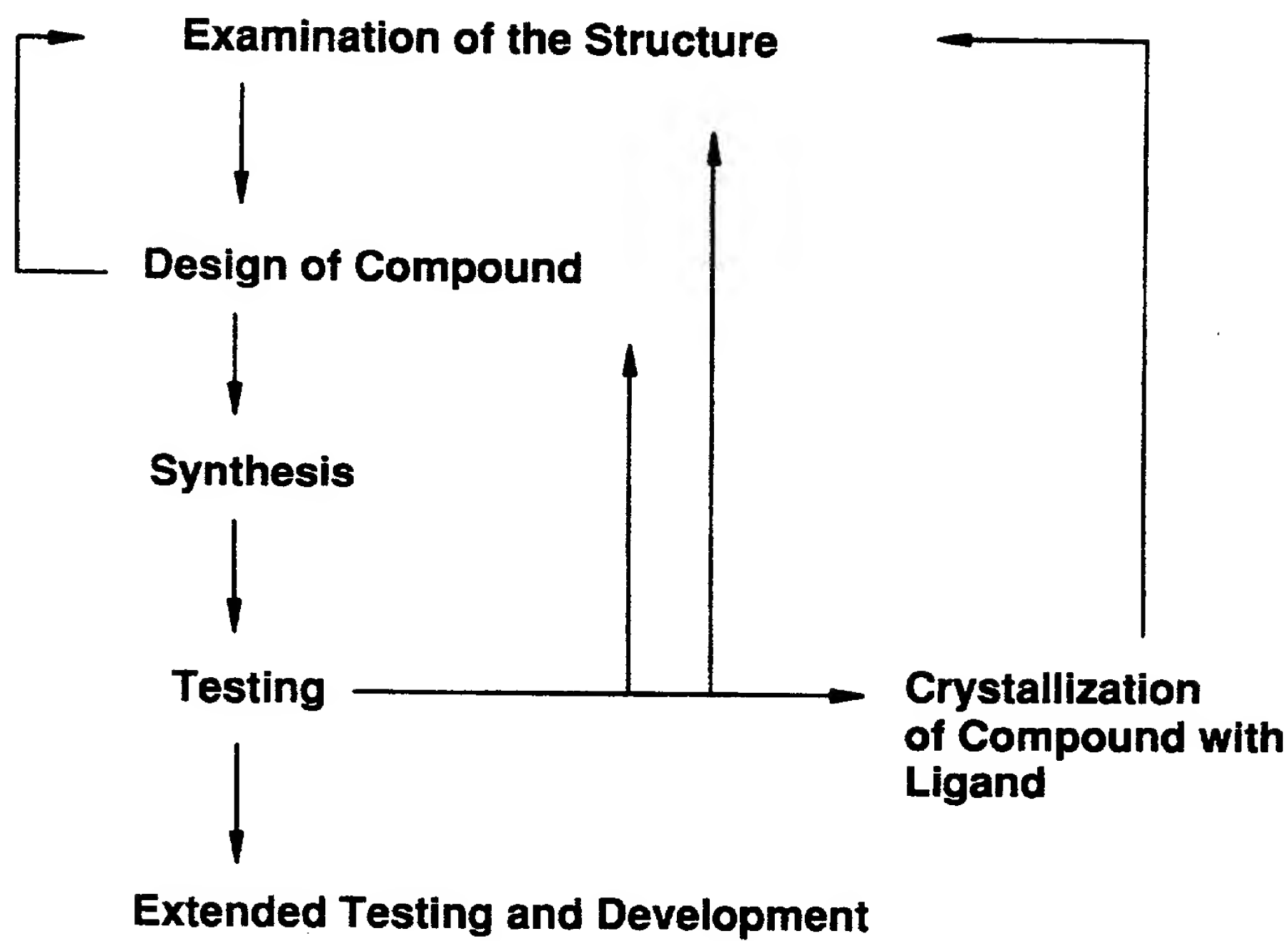


FIG.2

DOMAINS :	NH <sub>2</sub> - TERMINAL	DNA BINDING	LIGAND BINDING
HOMOLOGY :	Hypervariable	> 40%	About 20%
FUNCTION :	Transactivation	DNA Binding Dimerization	LIGAND Binding Dimerization Transactivation Nuclear translocation Hsp binding







	181		240
rTRa1pha	.....	.....	.....
hTRa1pha	.....	.....	.....
hTRbeta	.....	.....	.....
hRAa1pha	.....	.....	.....
hRAa1gamma	.....	.....	.....
hRXa1pha	.....	.....	.....
hRXRbeta	.....	.....	.....
hPPARa1pha	.....	.....	.....
hPPARbeta	.....	.....	.....
hPPARgamma	.....	.....	.....
hVDR	.....	.....	.....
hER	.....	.....	.....
hGR	QDPDLKAVS	LSMGLYMGET	ETKVMGNDLG FPQQQISLS SGETDLKLE ESTANLNRS.
hPR	AHKVLPKGLS	PARQLLPAS	ESPHWSGAPV KPSPQAAVE VEEEDSSESE ESACPILKKGK
hMR	VMRAIVK..S	PIMCHEKSPS	VCSPLNHTSS VCSPAGINSV SSTASFGSF PVHSPITQGT
hAR	.....	.....	.....

FIG.3D























	781		840
hTRAlpha	.....	.SMPDGDKVD LEAFSEFTKI	ITPAITRVVD FAKKLPMFSE LPCEDQIILL
hTRAlpha	.....	.SMPDGDKVD LEAFSEFTKI	ITPAITRVVD FAKKLPMFSE LPCEDQIILL
hTRbeta	.....	.NAPEGGKVD LEAFSHFTKI	ITPAITRVVD FAKKLPMFCE LPCEDQIILL
hRARalpha	.....	.....SLD IDLWDKFSEL	STKCIKTVE FAKQLPGFTT LTIADQITLL
hRARgamma	.....	.....QLD LGLWDKFSEL	ATKCIKIVE FAKRLPGFTG LSIADQITLL
hRXRalpha	.....	.NDPVTNICQ A.....	ADKQLFTLVE WAKRIPHFSE LPLDDQVILL
hRXRbeta	.....	.NDPVTNICQ A.....	ADKQLFTLVE WAKRIPHFSS LPLDDQVILL
hPPARalpha	.....	.....KEVE VRIFHCCQCT	SVEVTTELTE FAKAIPAFAN LDLNDQVTLL
hPPARbeta	.....	.....VHVEYRCQCT	TVETVRELTE FAKSIPSFSS LFLNDQVTLL
hPPARgamma	.....	.....IRIFQGCQFR	SVEAVQEITE YAKNIPGFIN LDLNDQVTLL
hVDR	.....	.....QLLNSQGQI	IATIGNPTA AIPSTASVLP KATVPLTLTK TTTQGPVGKV
hER	.....	.....YDPTRPFE	ASMGLLTNL ADRELVHMVN WAKRVPGFVD LTLHDQVHLL
hGR	.....	.....CYDSSVPDST	WRIMTTLNML GGRQVIAAVK WAKAIPGFRN LHLDDQMTLL
hPR	.....	.....GHDNTKPDTS	SSLTSLNQL GERQLLSVK WSKSLPGFRN LHIDDQITLI
hMR	.....	.....CYDSSKPDTA	ENLSTLNRL AGKQHIQVVK WAKVLPGEKN LPLEDQITLI
hAR	.....	.....GHDNNQPSF	AALLSSLNEL GERQLVHVVK WAKALPGFRN LHVDDQMAVI

FIG. 3N



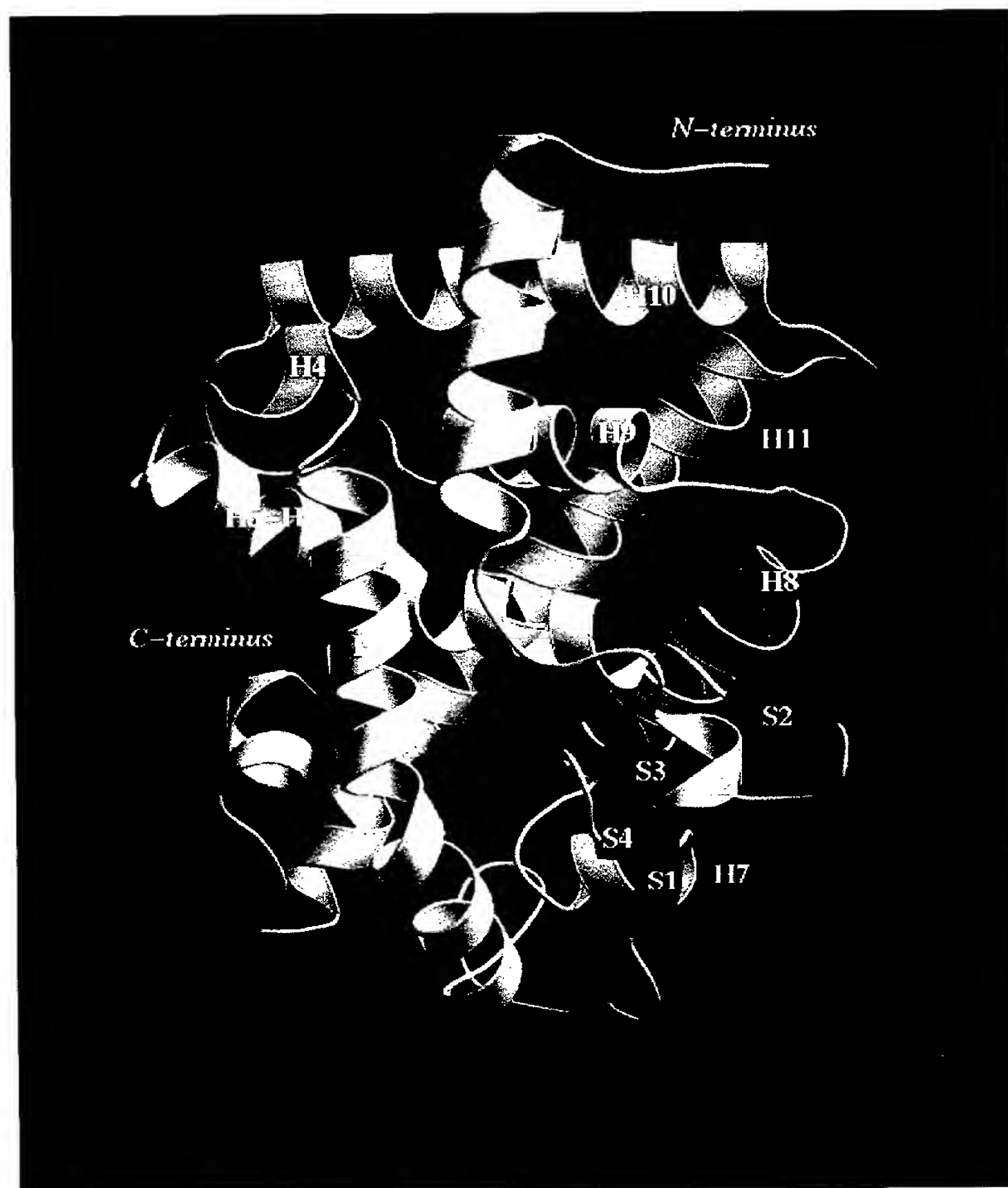
	841	900
rTRa1pha	KGCCMEIMSL RAAVRY..DP ESDTLTISGE MTKRKQLK..N..GGLGV VSDAIFELGK	
hTRa1pha	KGCCMEIMSL RAAVRY..DP ESDTLTISGE MAVKREQLK..N..GGLGV VSDAIFELGK	
hTRbeta	KGCCMEIMSL RAAVRY..DP ESETLTNGE MAVIRGQLK..N..GGLGV VSDAIFDLGH	
hRAa1pha	KAACLDILIL RICTRY..TP EQDTMTFSDG LTLNRTQMH..N..AGFGP LTDLVFAFAN	
hRAArgamma	KAACLDILML RICTRY..TP EQDTMTFSDG LTLNRTQMH..N..AGFGP LTDLVFAFAG	
hRXRa1pha	RAGWNELLIA SFSHRS..IA VKDGILLATG LHVHRNSAH..S.AGVGAI FDRVLTTELVS	
hRXRbeta	RAGWNELLIA SFSHRS..ID VRDGILLATG LHVHRNSAH..S.AGVGAI FDRVLTTELVS	
hPPARa1pha	KYGVYEAIFA MLSSVM..NK DGMVAYGNG F.ITREFLK..SLRKPFC D IMEPKFDFAH	
hPPARbeta	KYGVHEAIFA MLASIV..NK DGLLVANGSG F.VTREFLR..SLRKPFS D IIEPKFEFAY	
hPPARgamma	KYGVHEIITYT MLASLM..NK DGVLISEGQG F.MTREFLK..SLRKPFG D FMEPKFEFAY	
hVDR	APSKVIAIPQ PSVVKPVTSL TAAGVIACGE MPTVGQLVNK PSAVKDEEAI NLEEIREFAK	
hER	ECAWLEILMI GLVWRS..ME HPGKLLFAPN LLDNRNQGK..C.VEGMVEI FDMLLAT.SS	
hGR	QYSWMFLMAF ALGWRSYRQS SANLLCFAPD LIINEQRMT..L.PCHYD QCKHMLYVSS	
hPR	QYSWMSLMVF GLGWRSYKHV SGQMLYFAPD LILNEQRMK..ESSFYS LCLTMWQIPQ	
hMR	QYSWMCLSSF ALSWRSYKHT NSQFLYFAPD LVFNEEKMH..Q.SAMYE LCQGMHQISL	
hAR	QYSWMGLMVF AMGWRSTNV NSRMLYFAPD LVFNEYRMH..KSRMYS QCVRMRHLSQ	

FIG.30





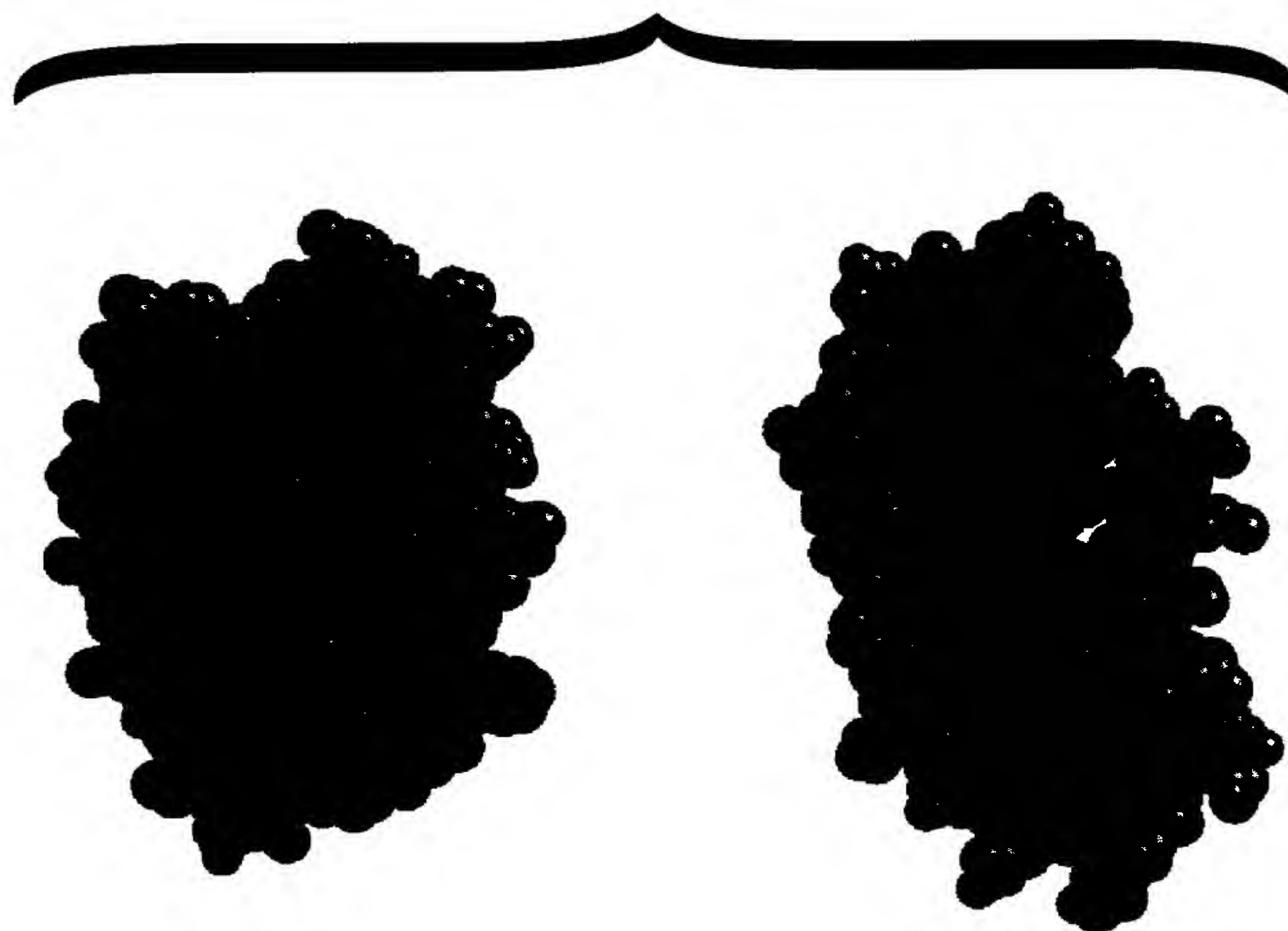




**FIG. 4**



**FIG. 5**



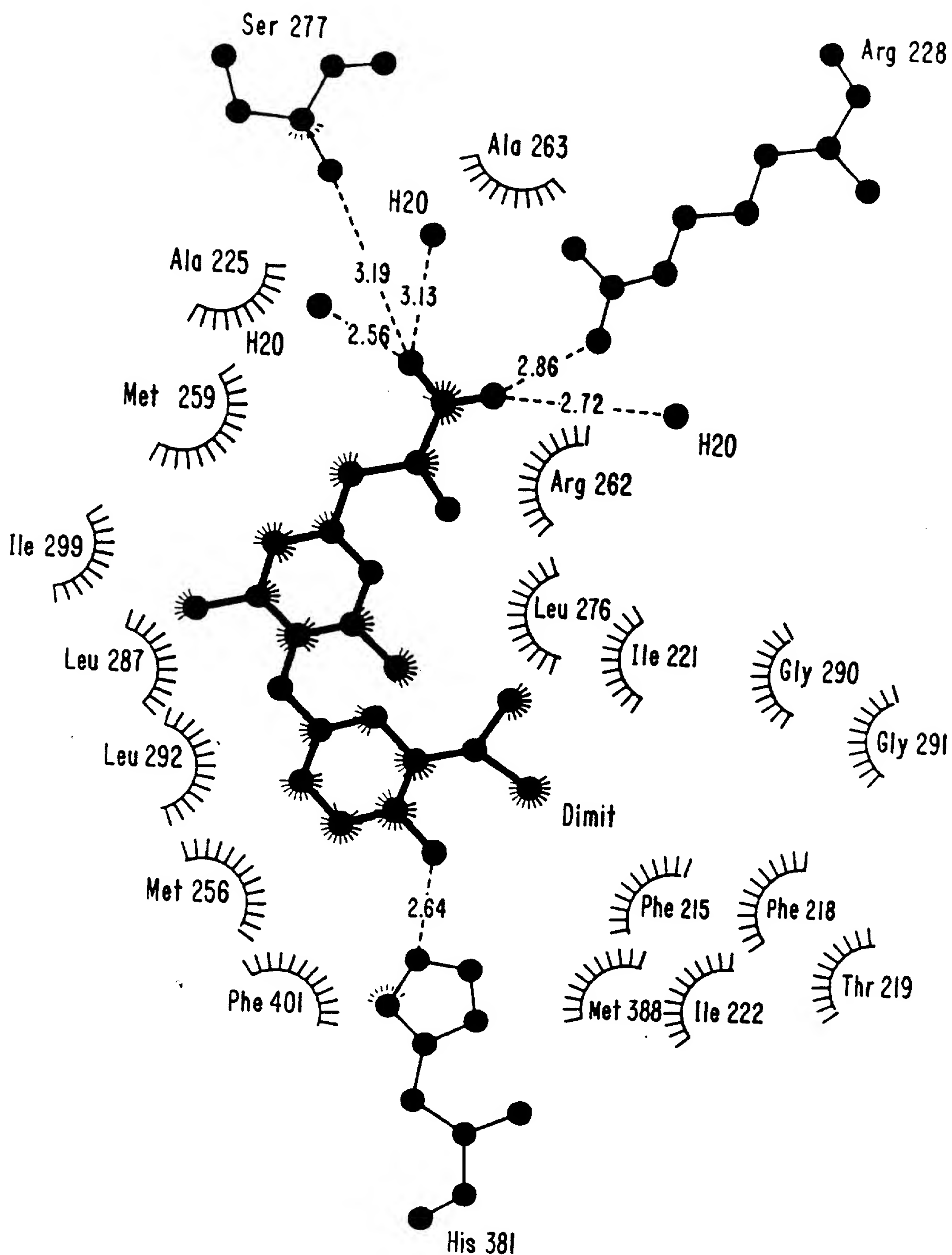
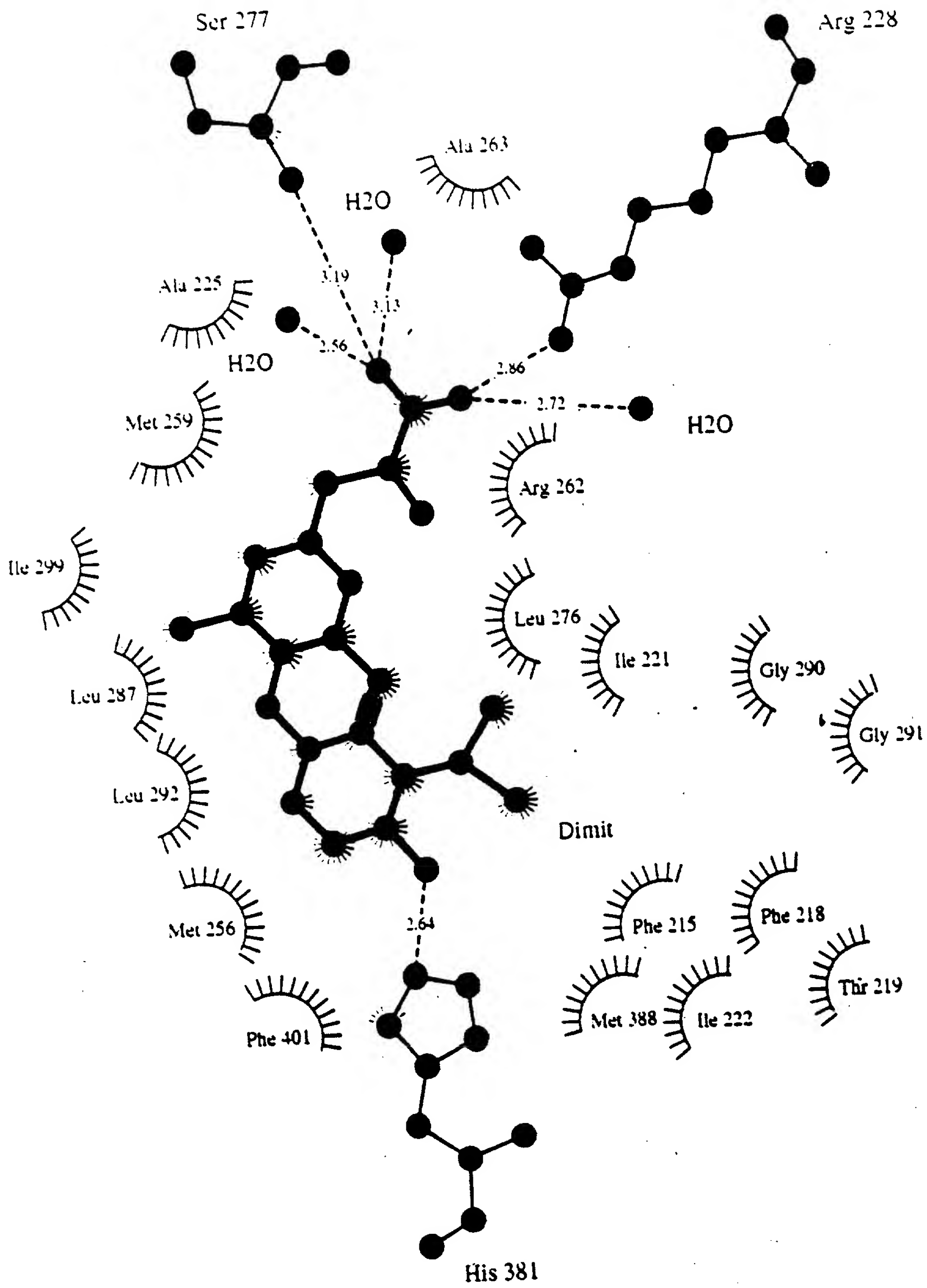


FIG.6



**Figure 6**

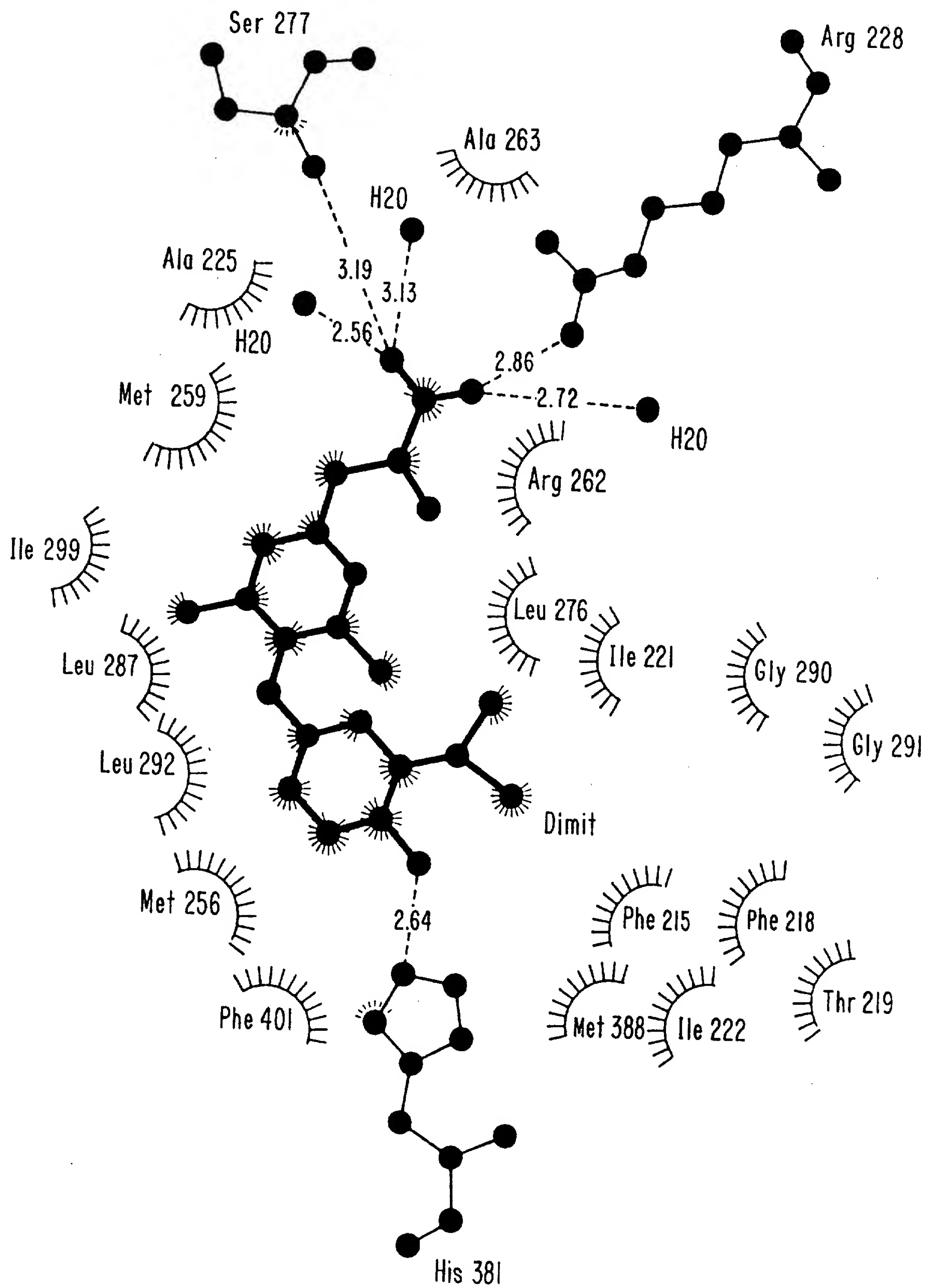
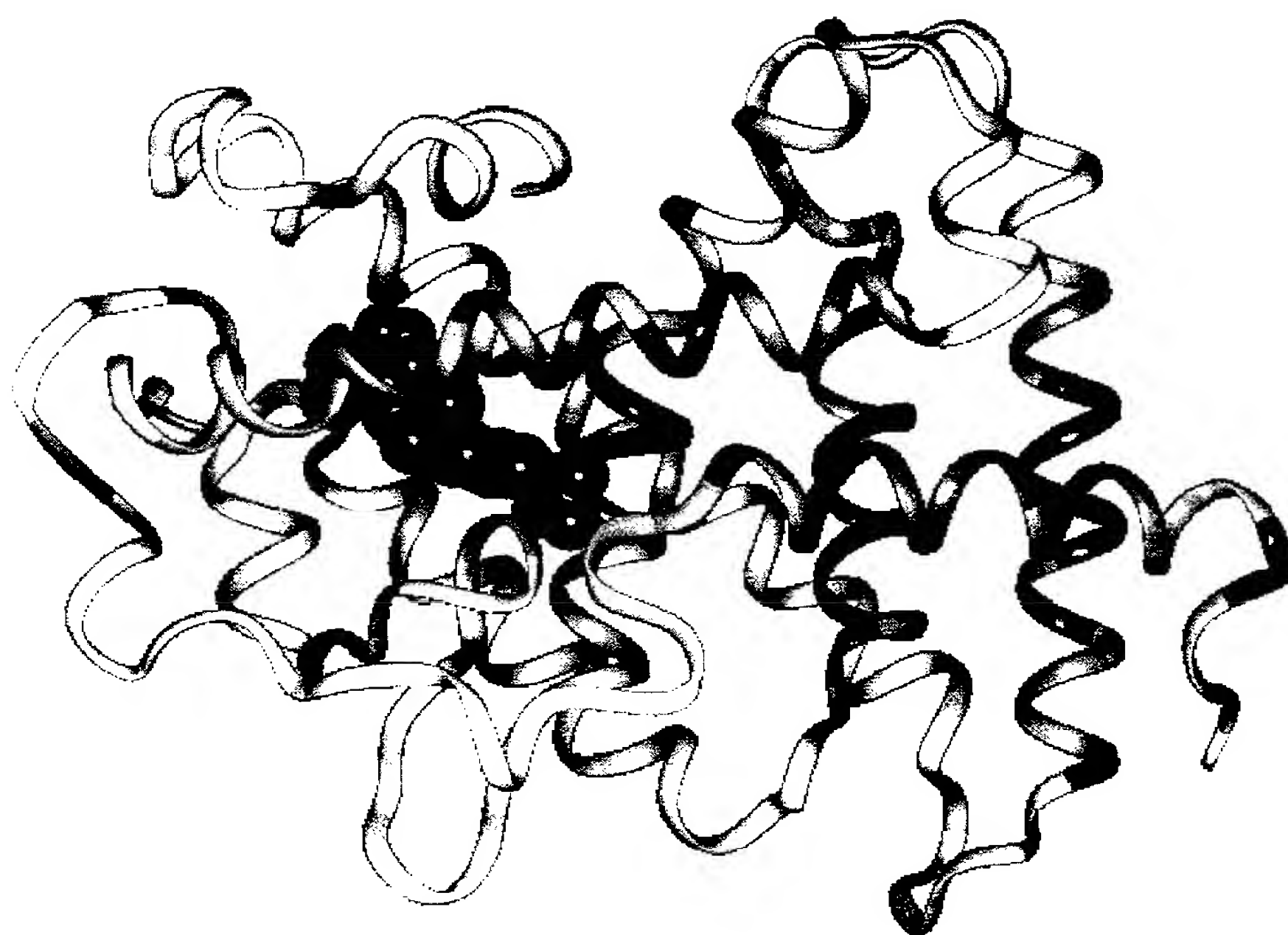


FIG.6

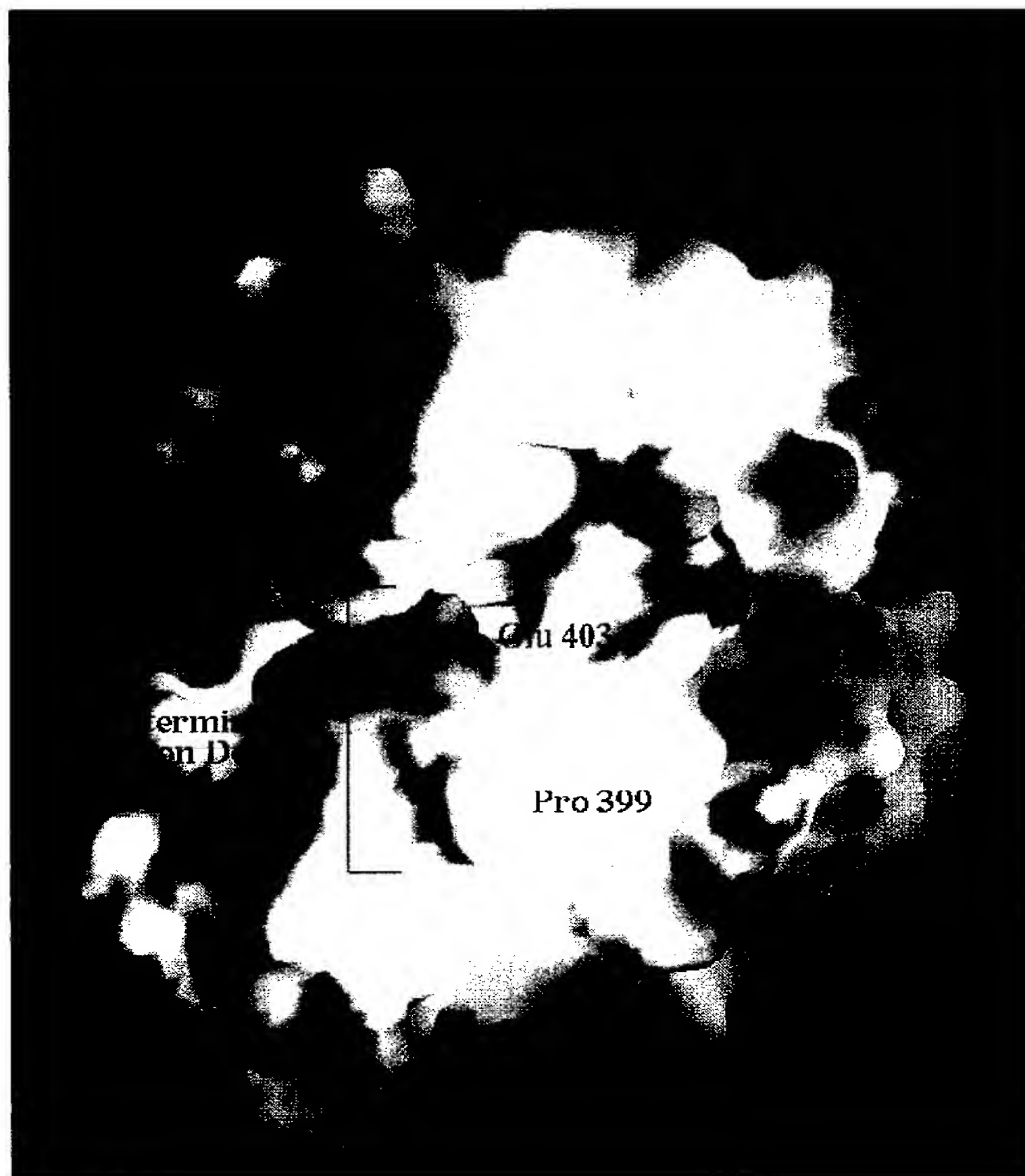


**FIG. 7**



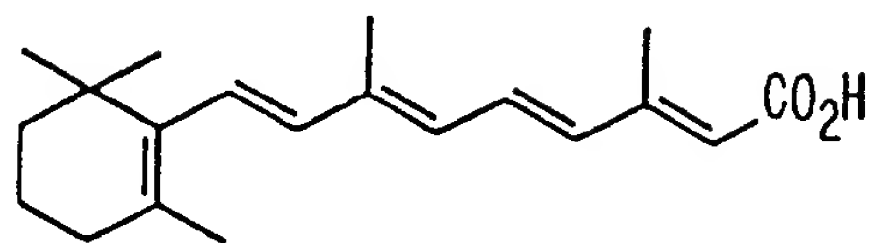


**FIG. 8**

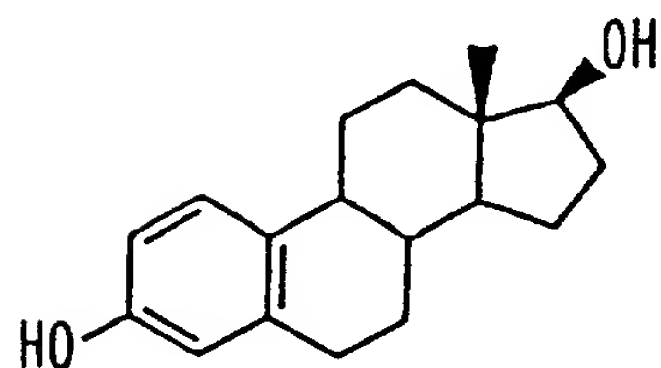


**FIG. 9**

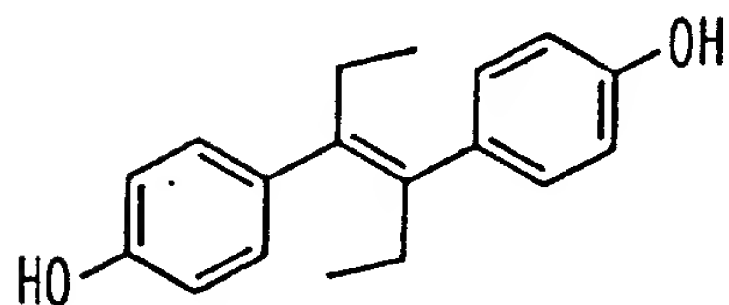
## AGONISTS



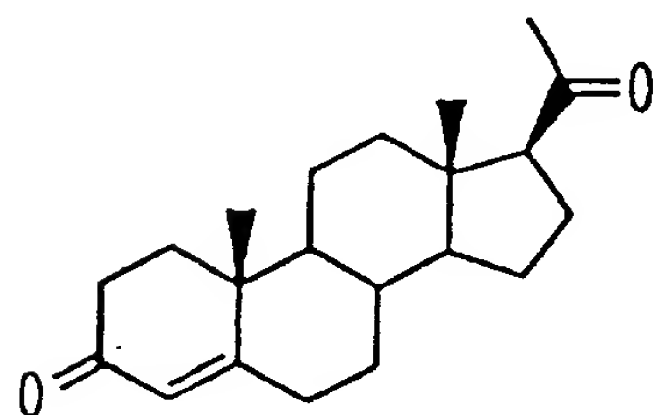
Retinoic Acid



Estradiol

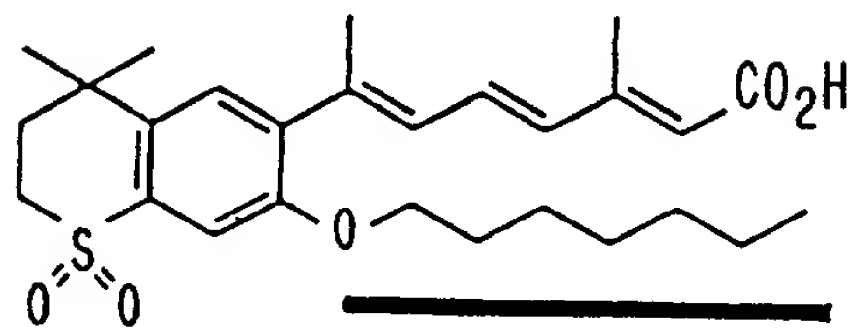


Diethylstilbestrol

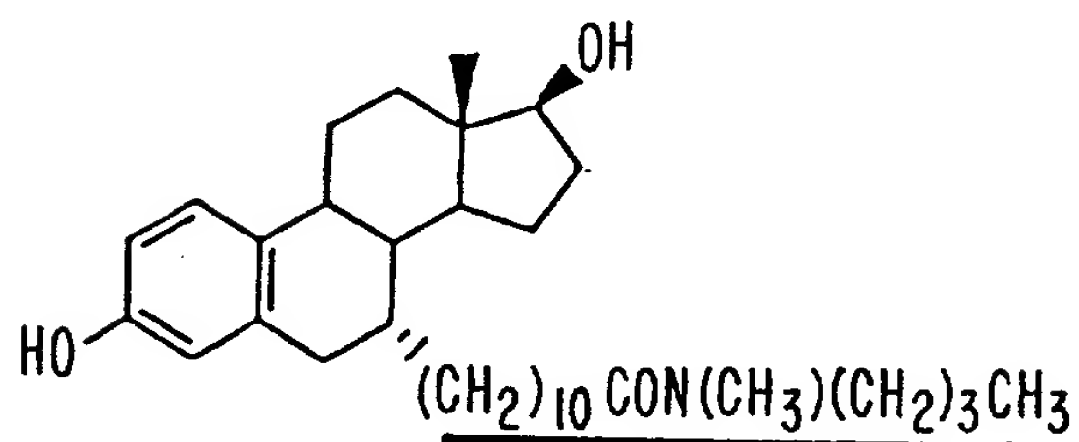


Progesterone

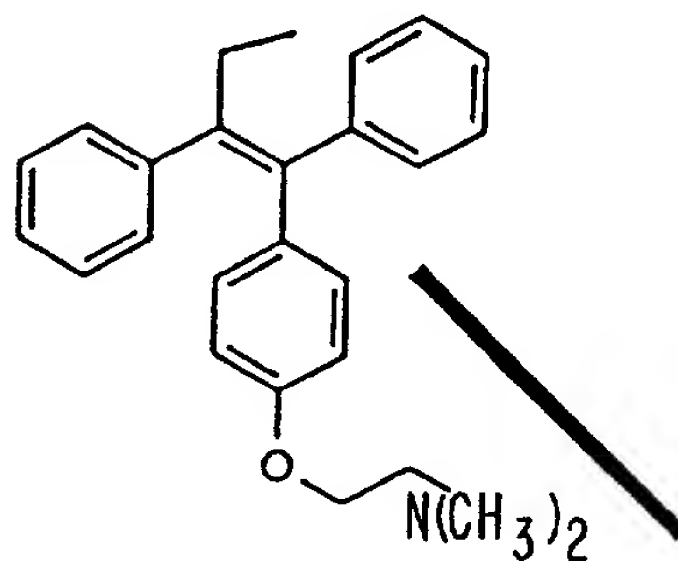
## ANTAGONISTS



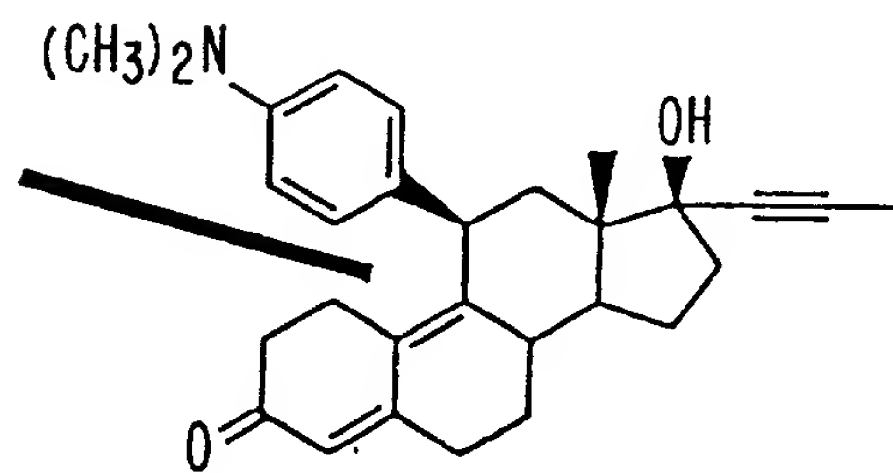
Ro 46-8515



ICI 164384



Tamoxifen



RU 486

FIG.10

shows position of extension group

Chemical reaction scheme showing the conversion of a substituted tyrosine derivative to an amide.

The reactant is a substituted tyrosine derivative, specifically 3,5-diiodo-4-(3,5-diiodo-4-hydroxyphenyloxy)phenyl-L-tyrosine. It features a central benzene ring with iodine atoms at the 3 and 5 positions, and a side chain consisting of a methylene group, a chiral center with an amino group ( $\text{NH}_2$ ) and a carboxylic acid group ( $\text{CO}_2\text{H}$ ), and an ether linkage to a 3,5-diiodo-4-hydroxyphenyl group.

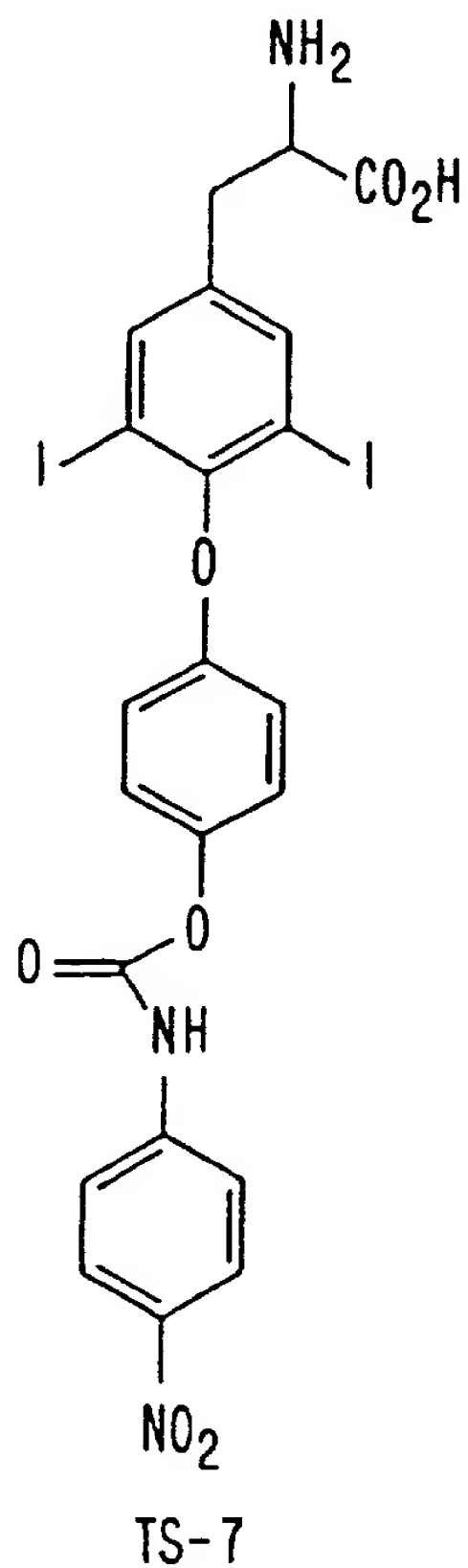
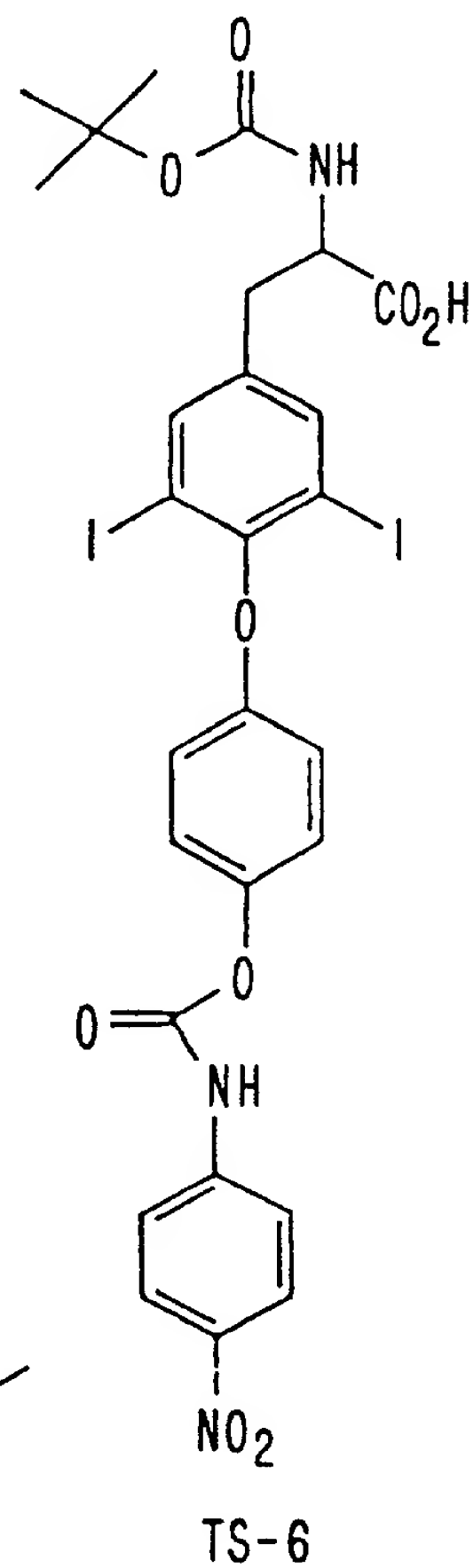
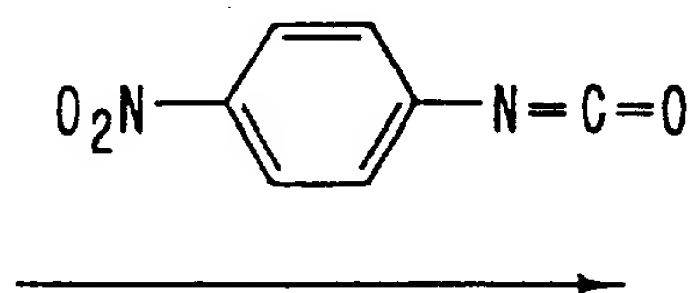
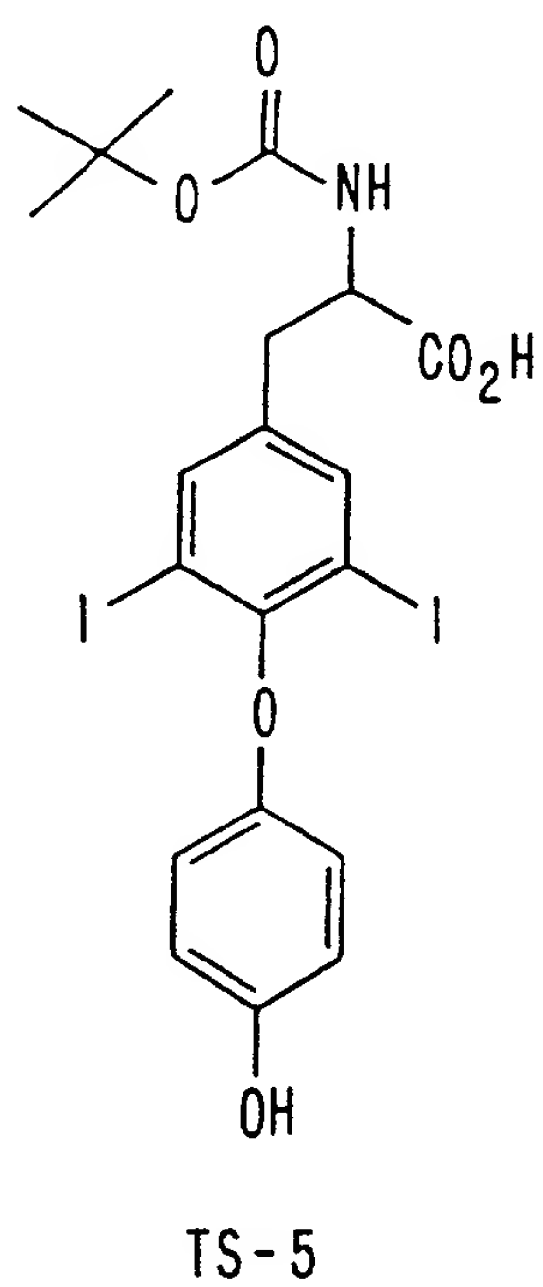
The reaction is catalyzed by  $\text{RCOX}$  (where  $\text{R}$  is a substituent and  $\text{X}$  is a leaving group).

The product is the corresponding amide, where the amino group of the tyrosine side chain has been converted to an amide group ( $\text{NH-C(=O)-R}$ ).

Compound	RCOX
TS1	$\text{Ph}_2\text{CHCO}_2\text{NHS}$
TS2	$\text{C}_{16}\text{H}_{33}\text{CO}_2\text{NHS}$
TS3	$\text{FMOC-Cl}$
TS4	$\text{tBOC}_2\text{O}$
TS5	$\text{tBOC}_2\text{O}$

FIG. 11

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100
1	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100
2	2	1	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100
3	3	2	1	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100
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TFA

FIG. 12



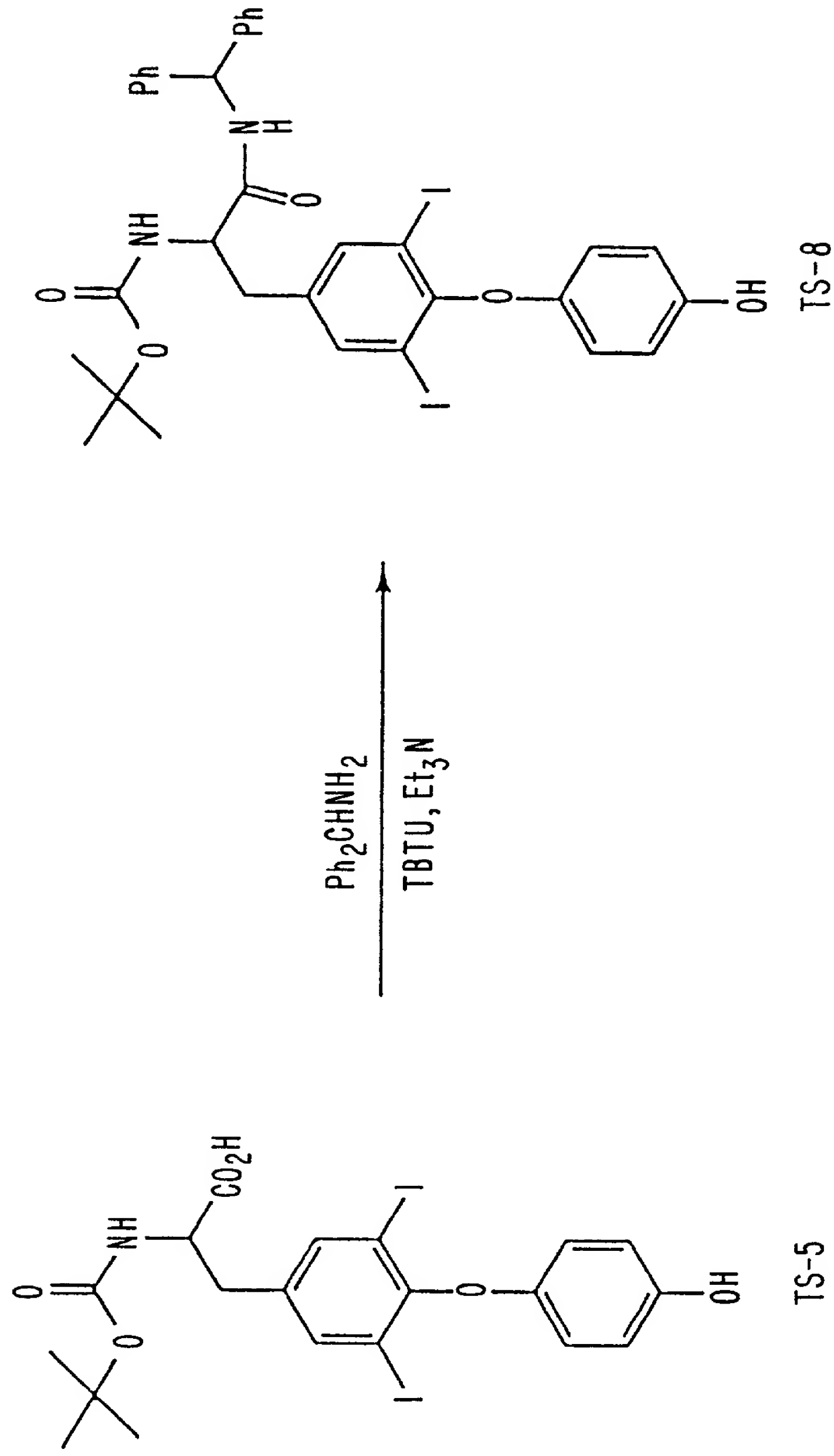


FIG.13

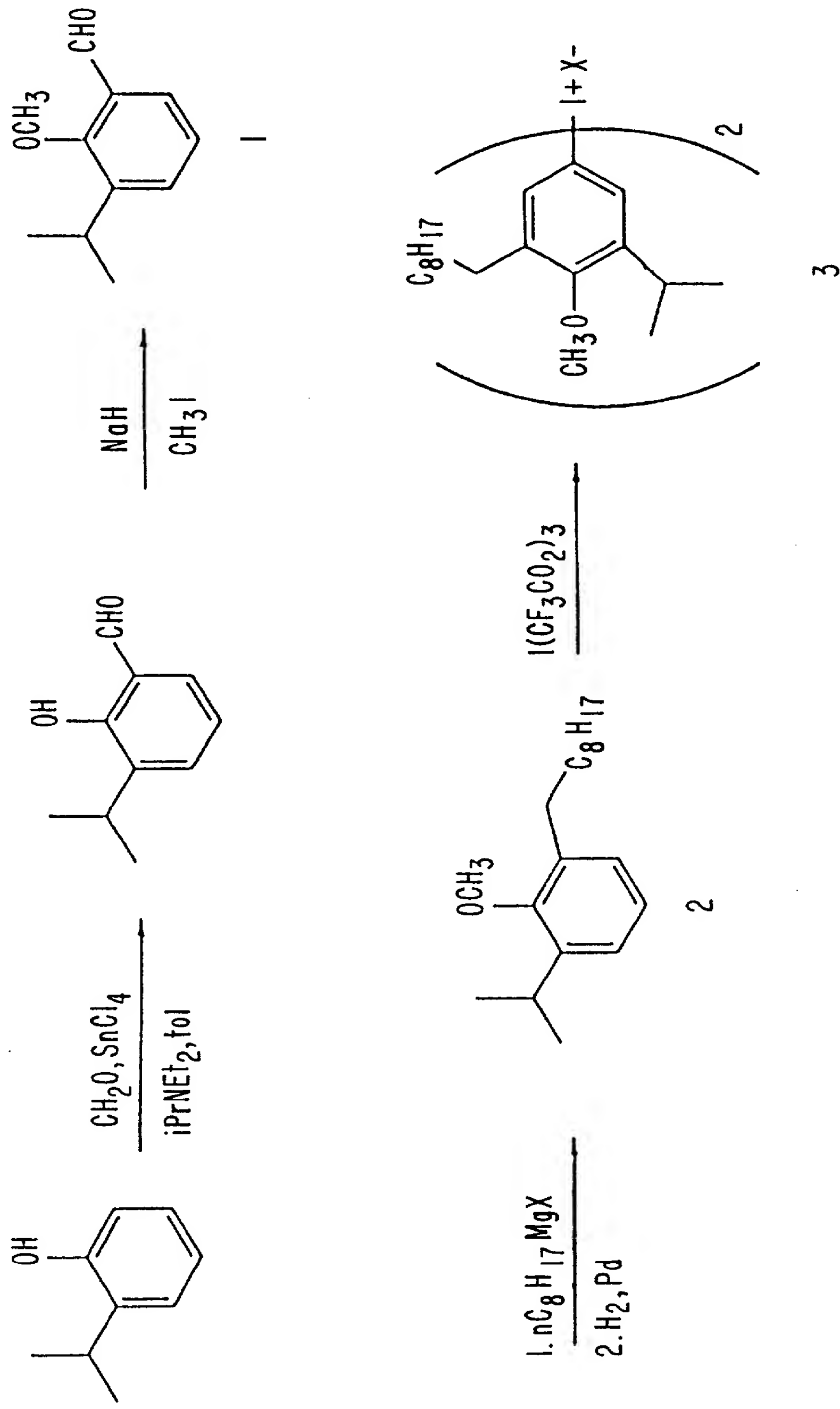


FIG.14A

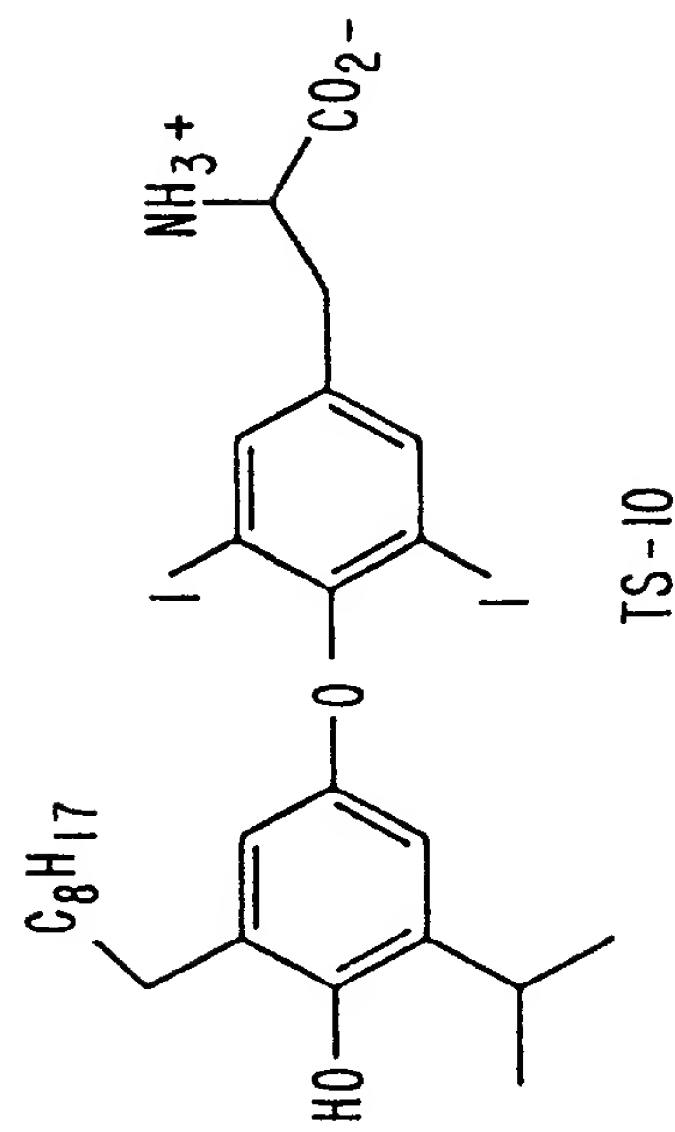
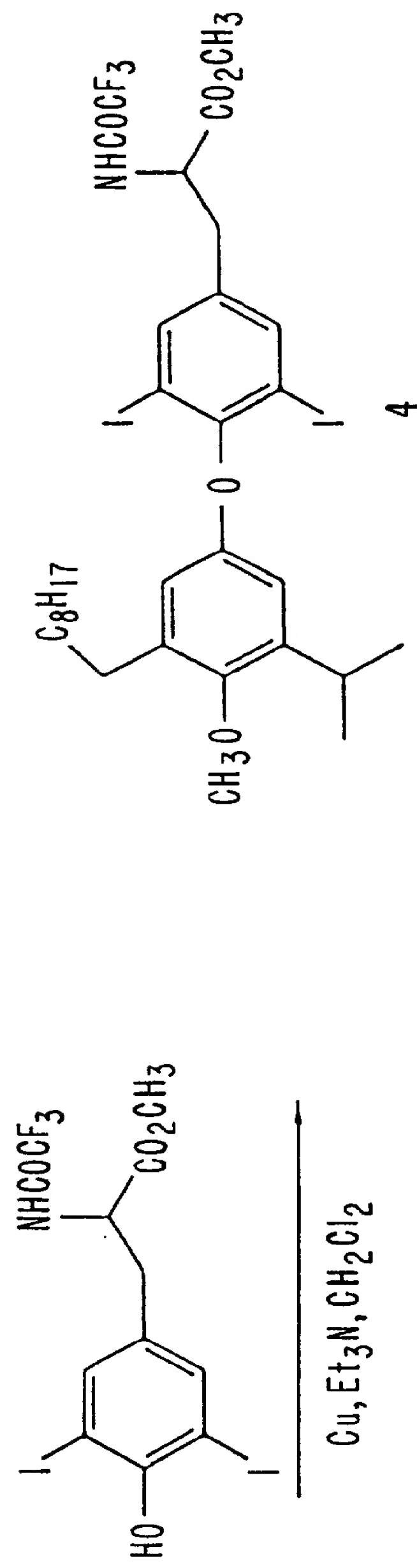
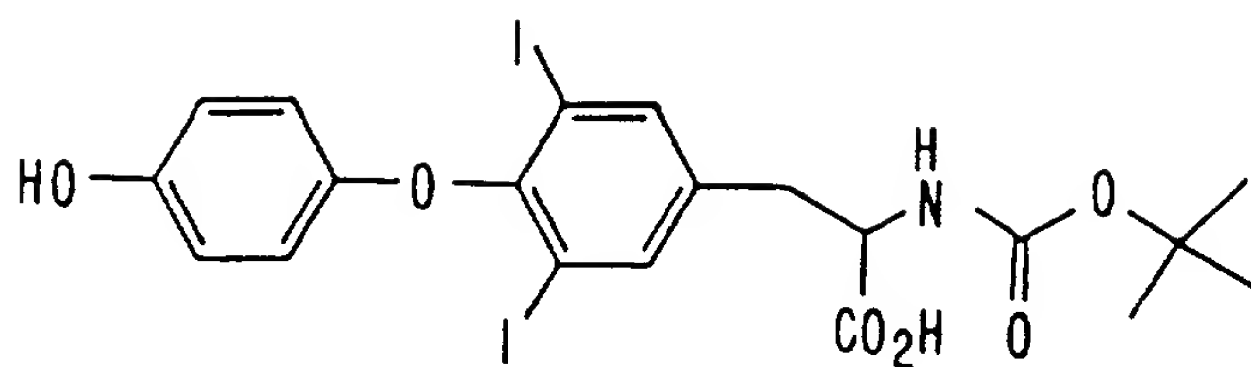
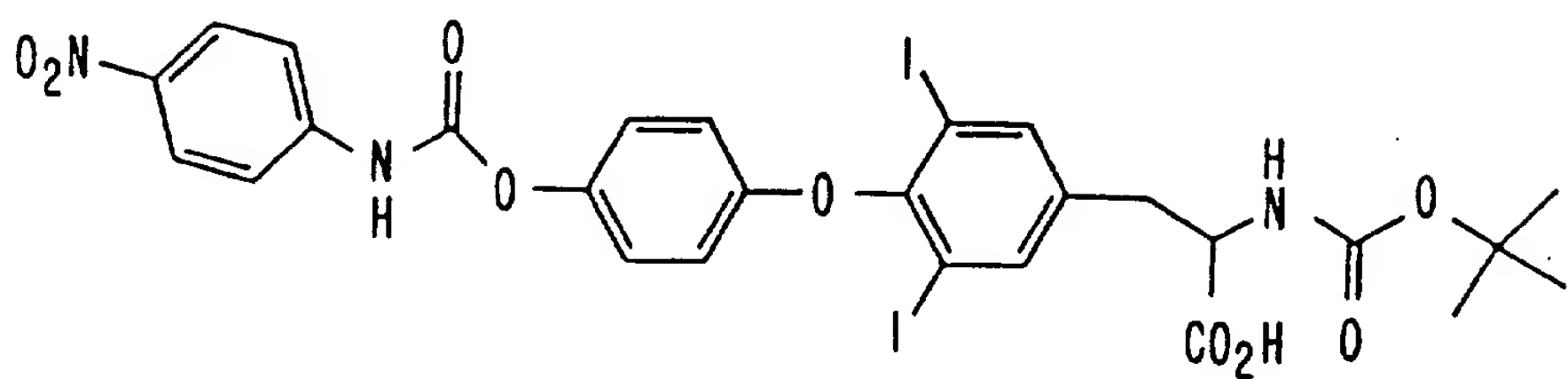


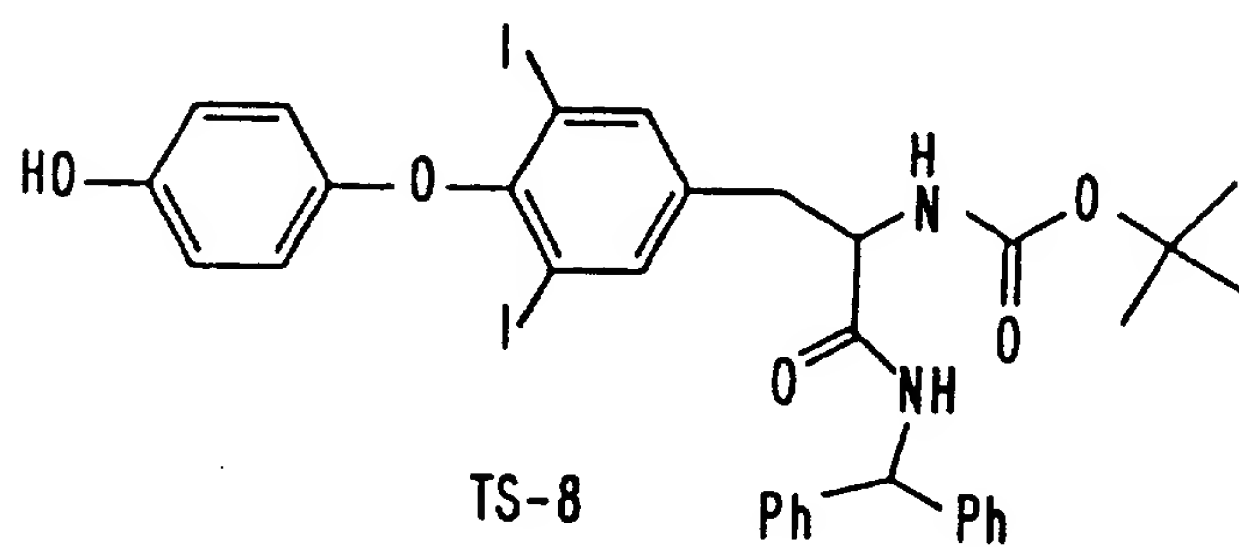
FIG.14B



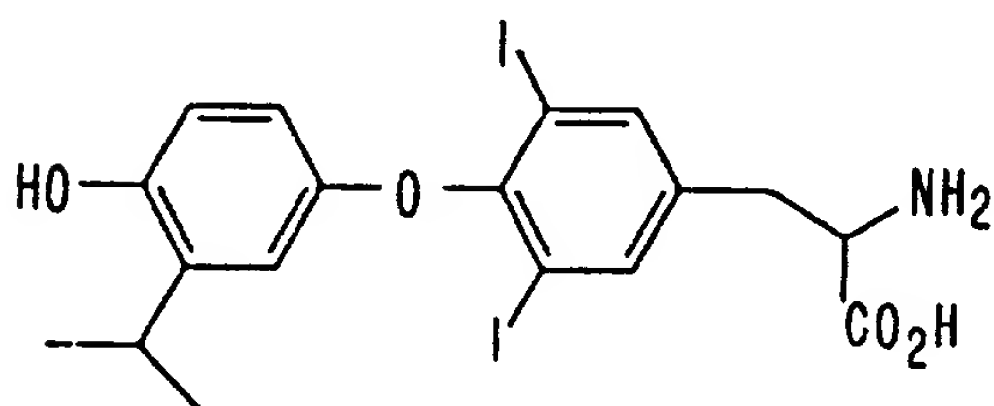
TS-5



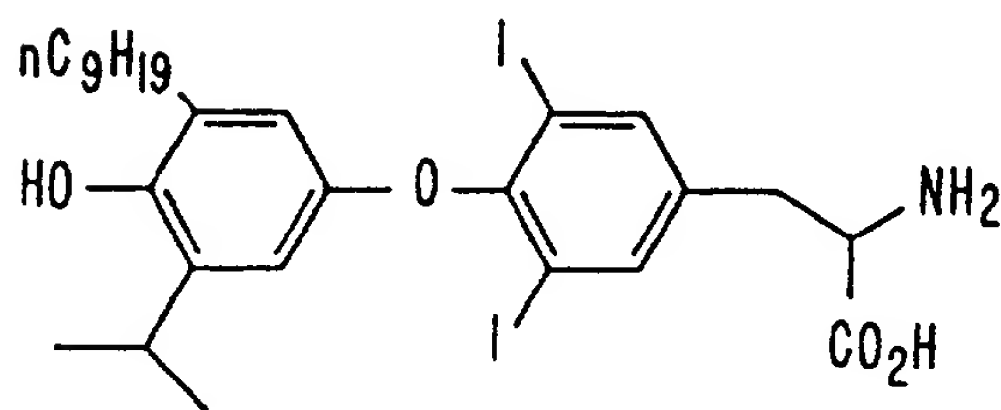
TS-6



TS-8



TS-9



TS-10

FIG.15

FIG.16

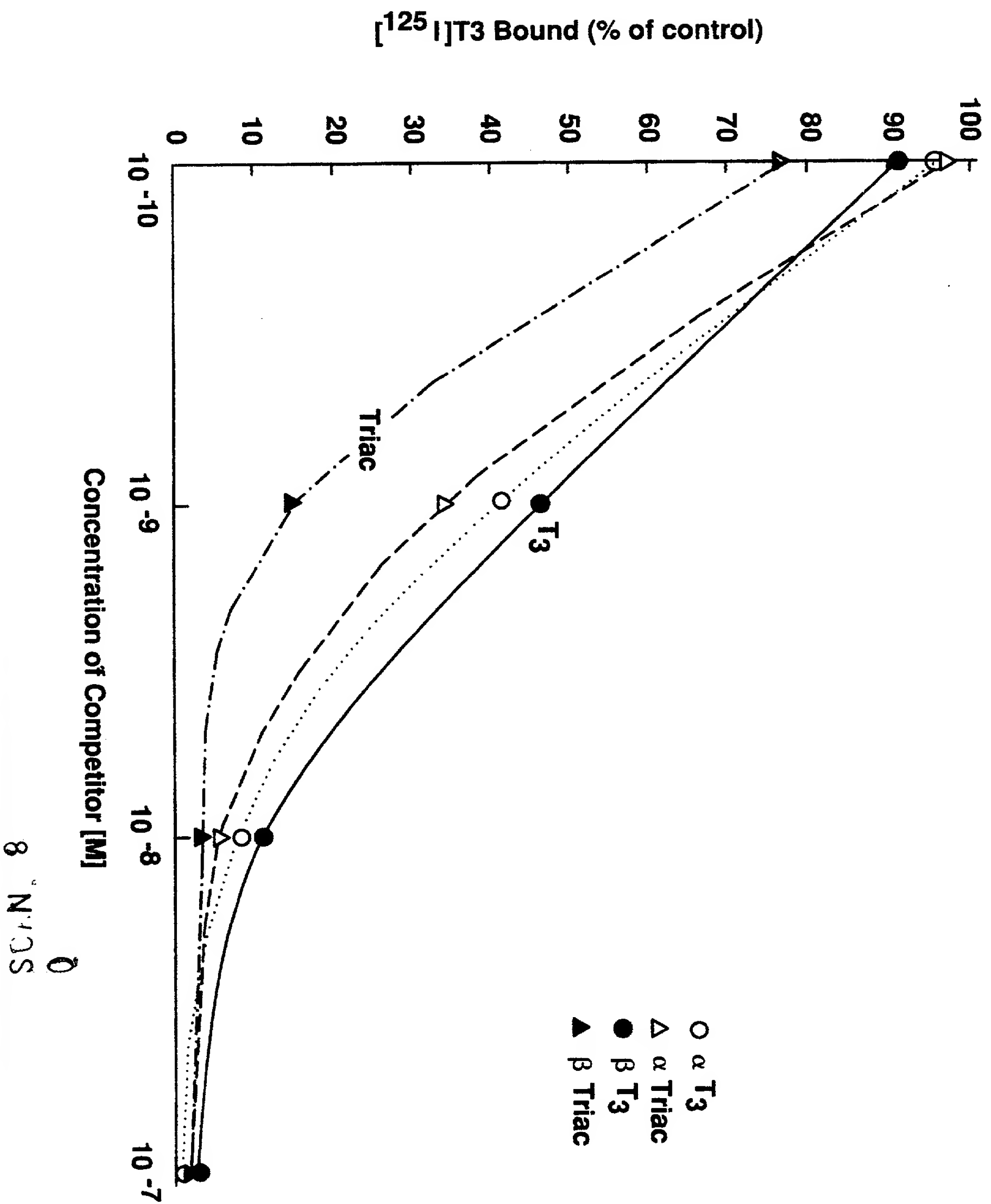




FIG.17A

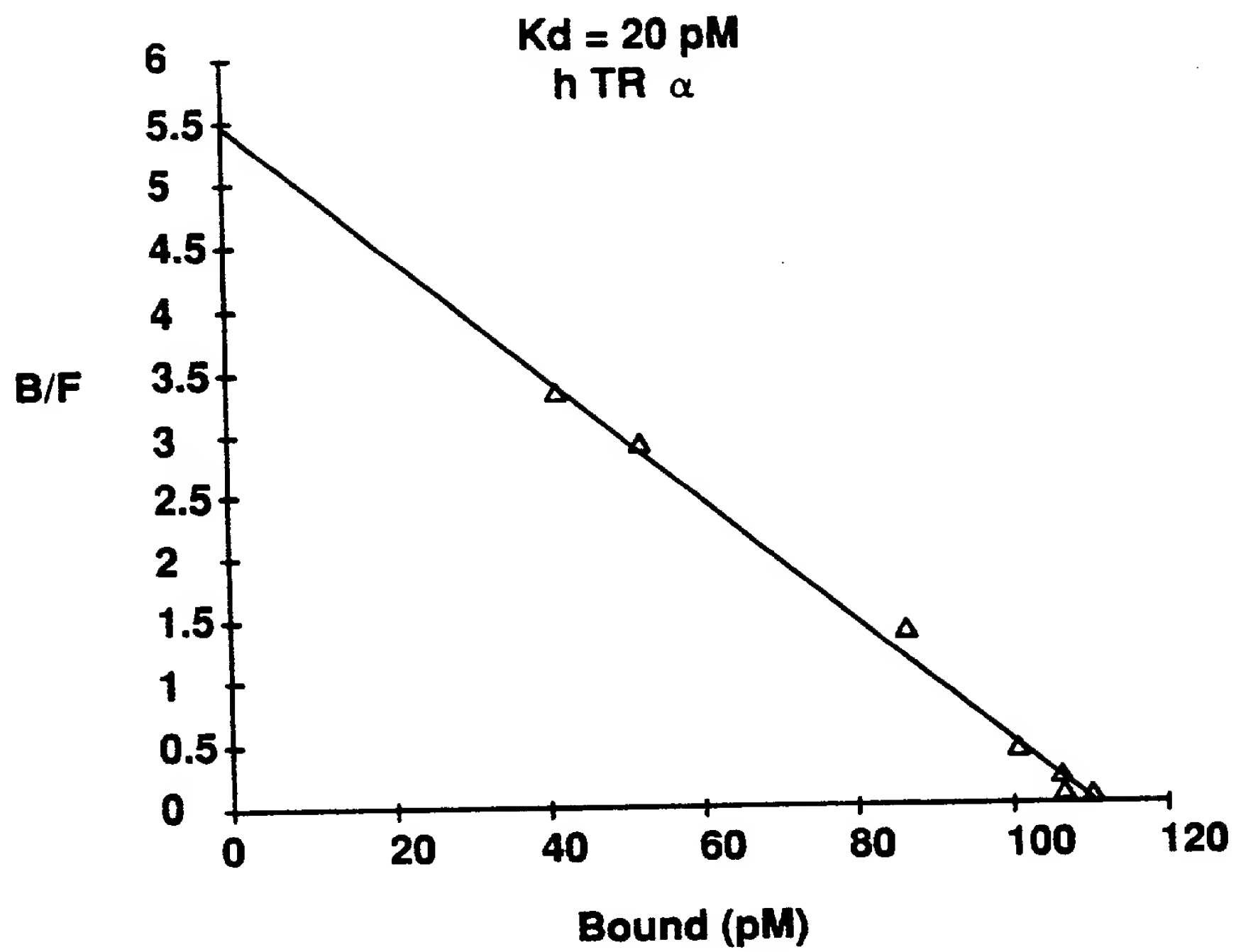
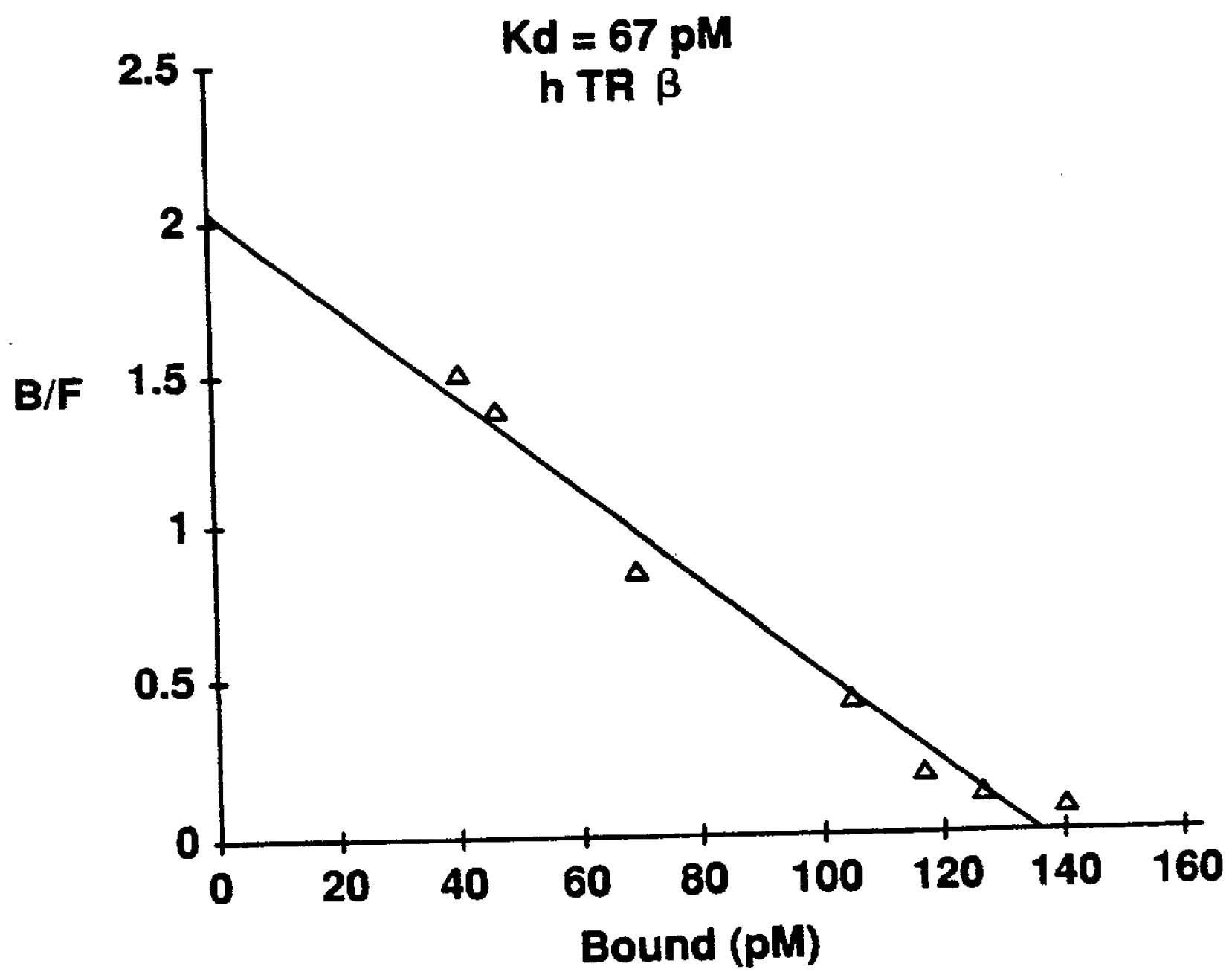


FIG.17B



**FIG. 18**

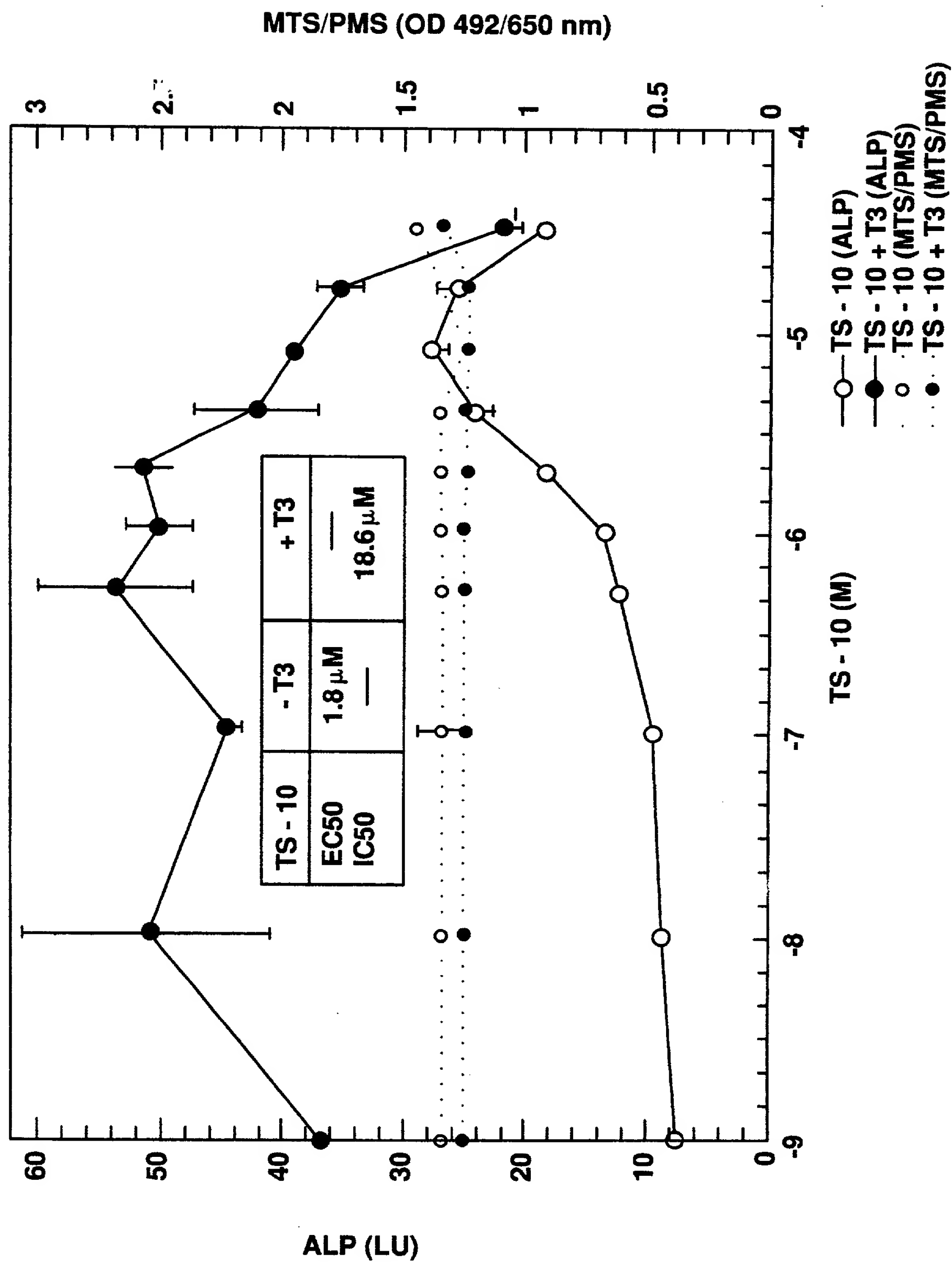
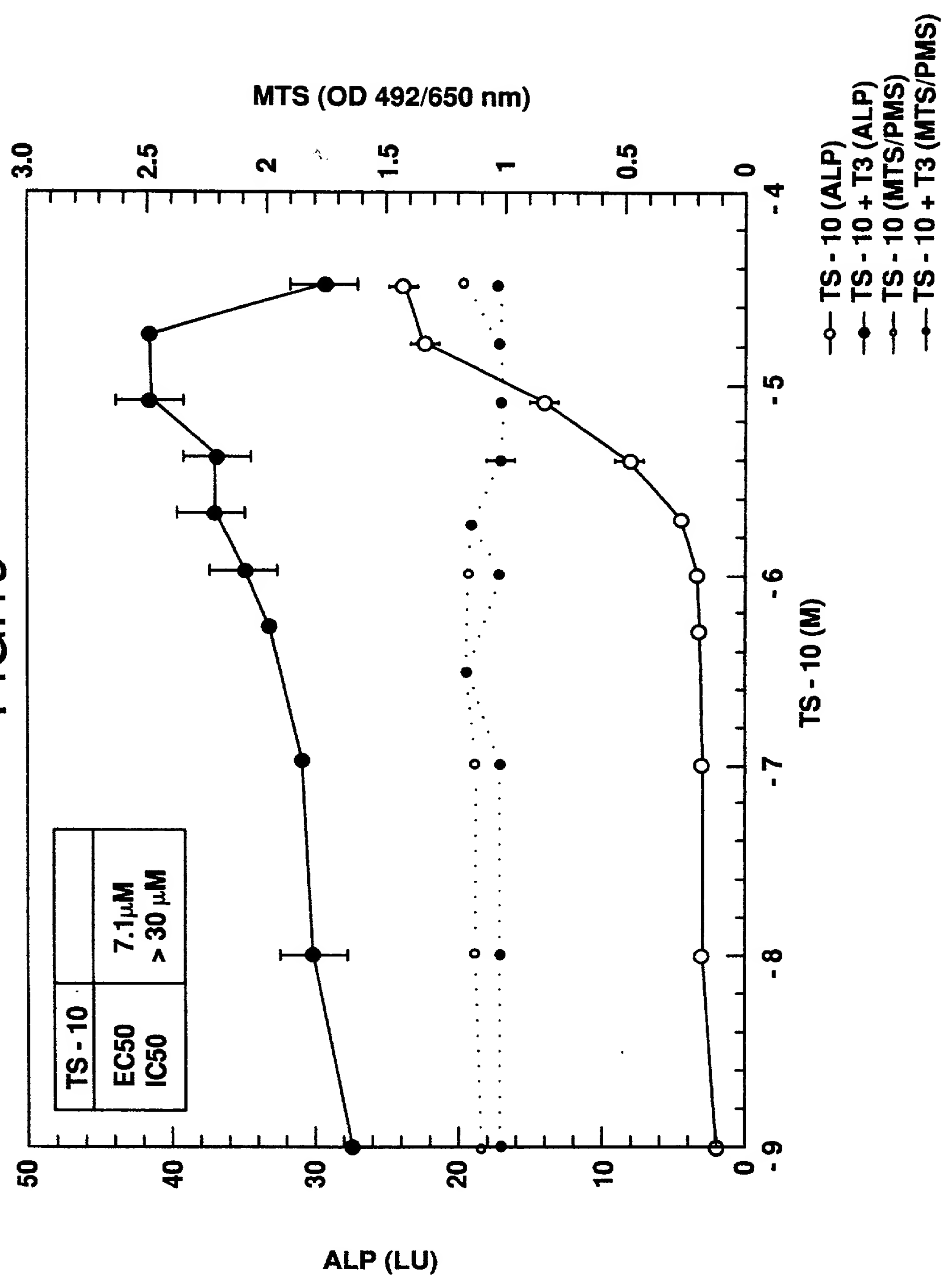
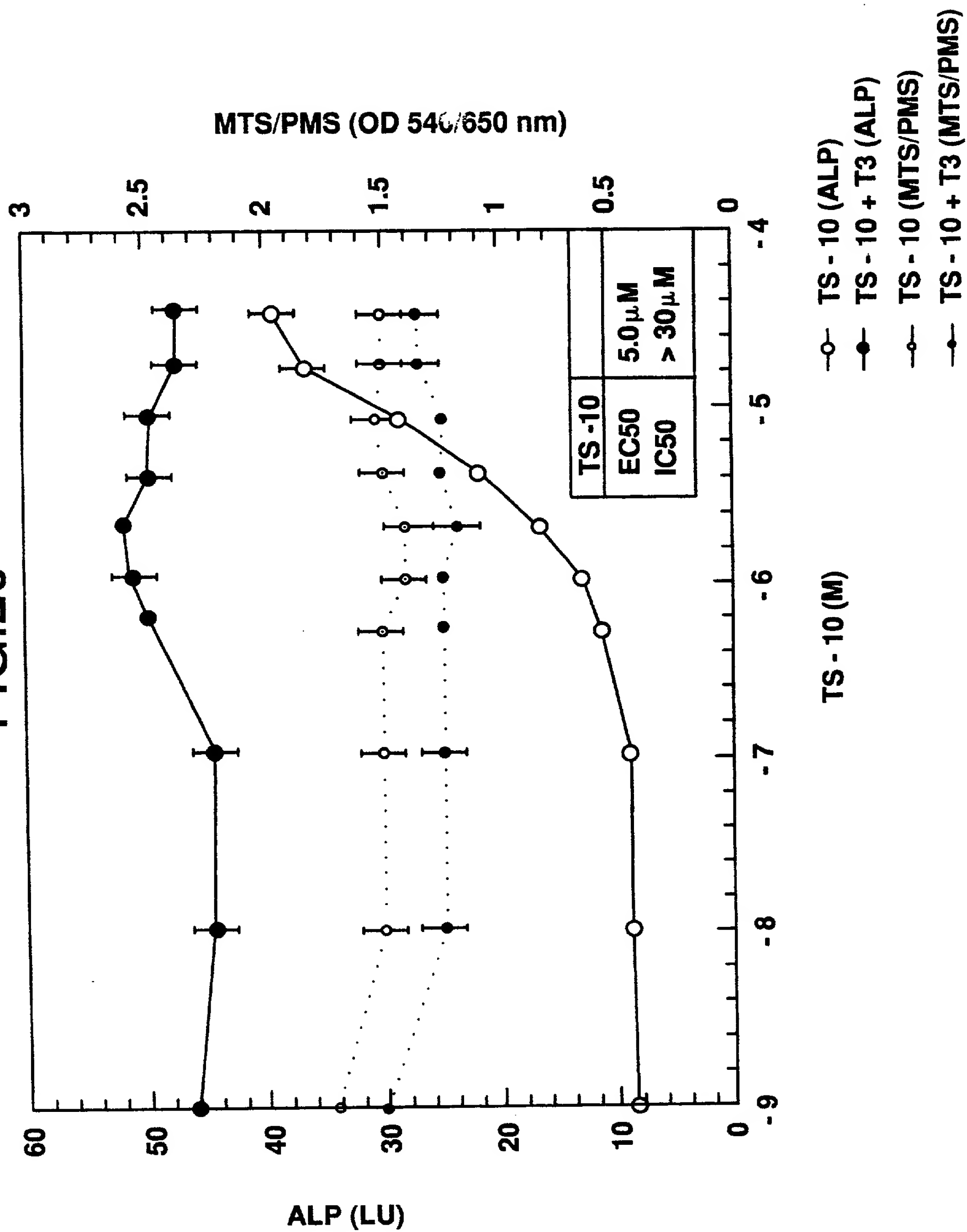
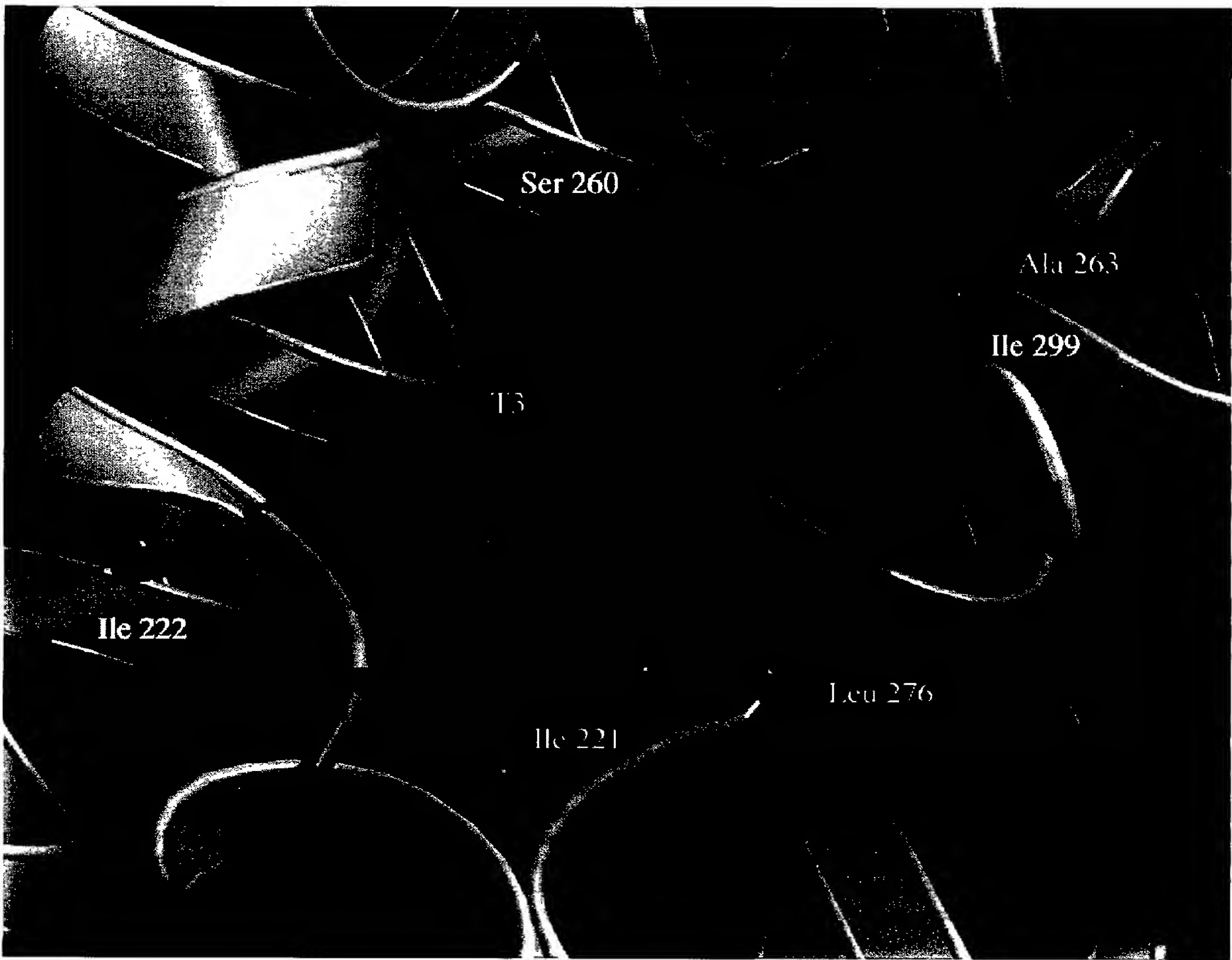


FIG.19

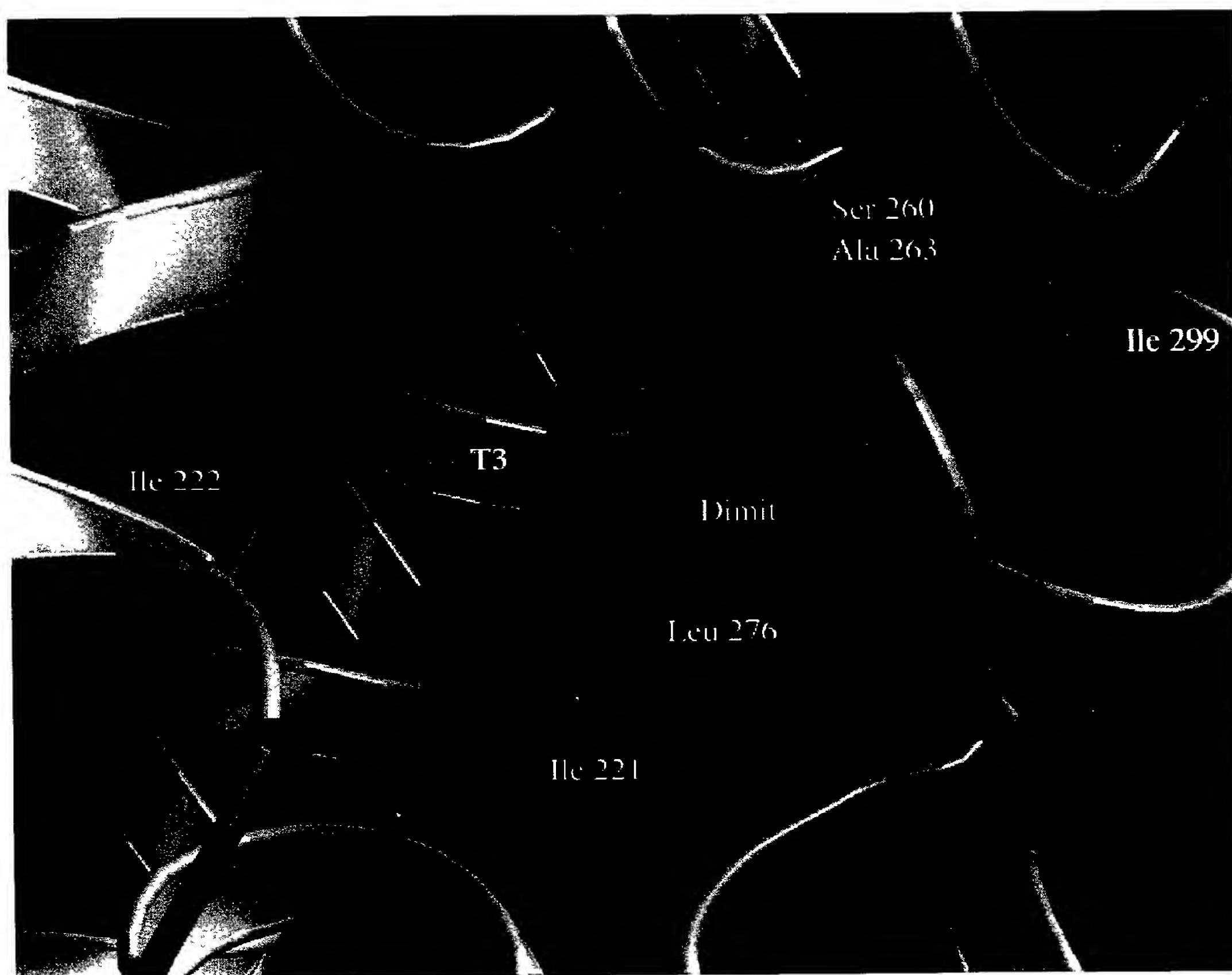




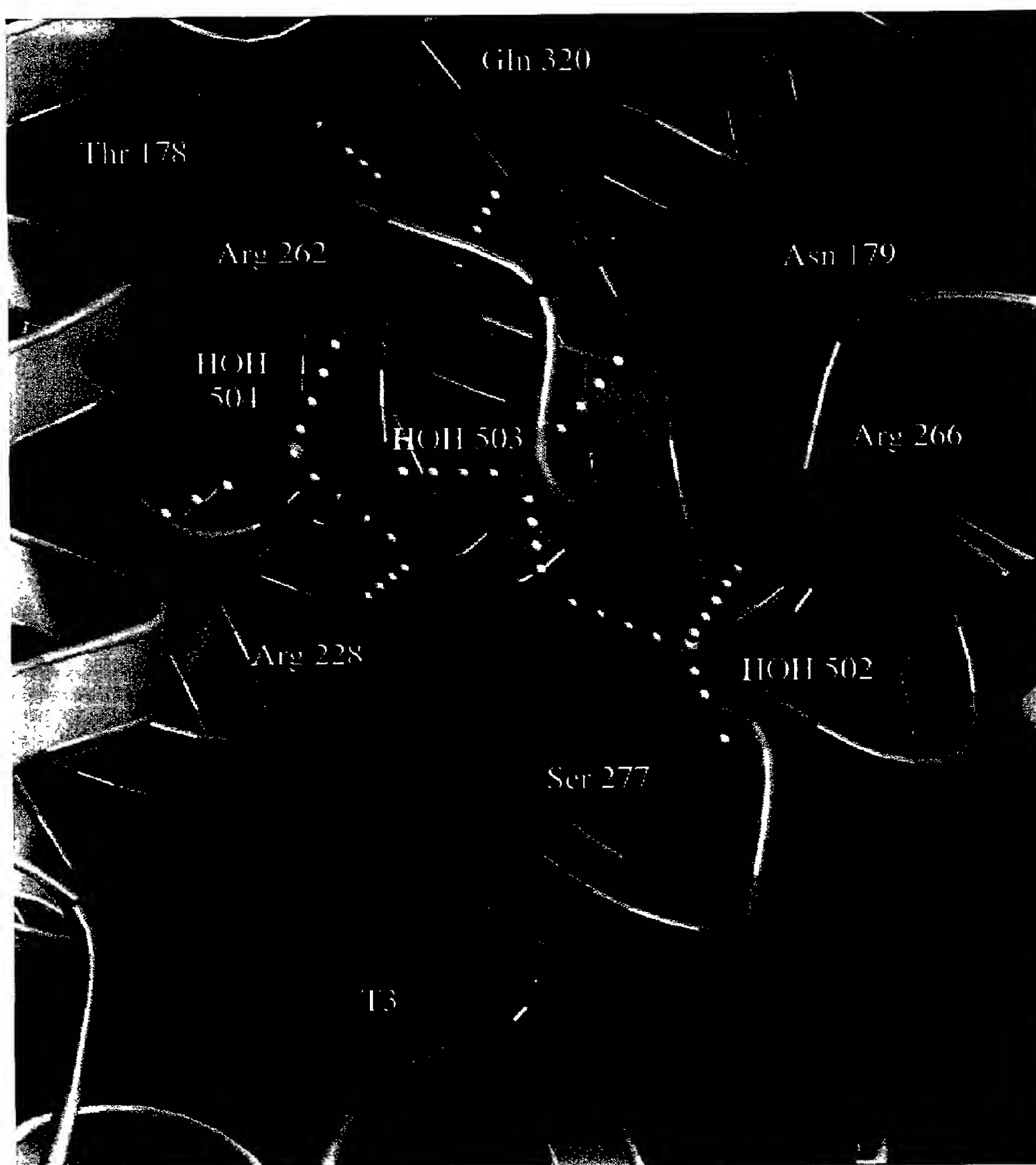


**FIG. 21**

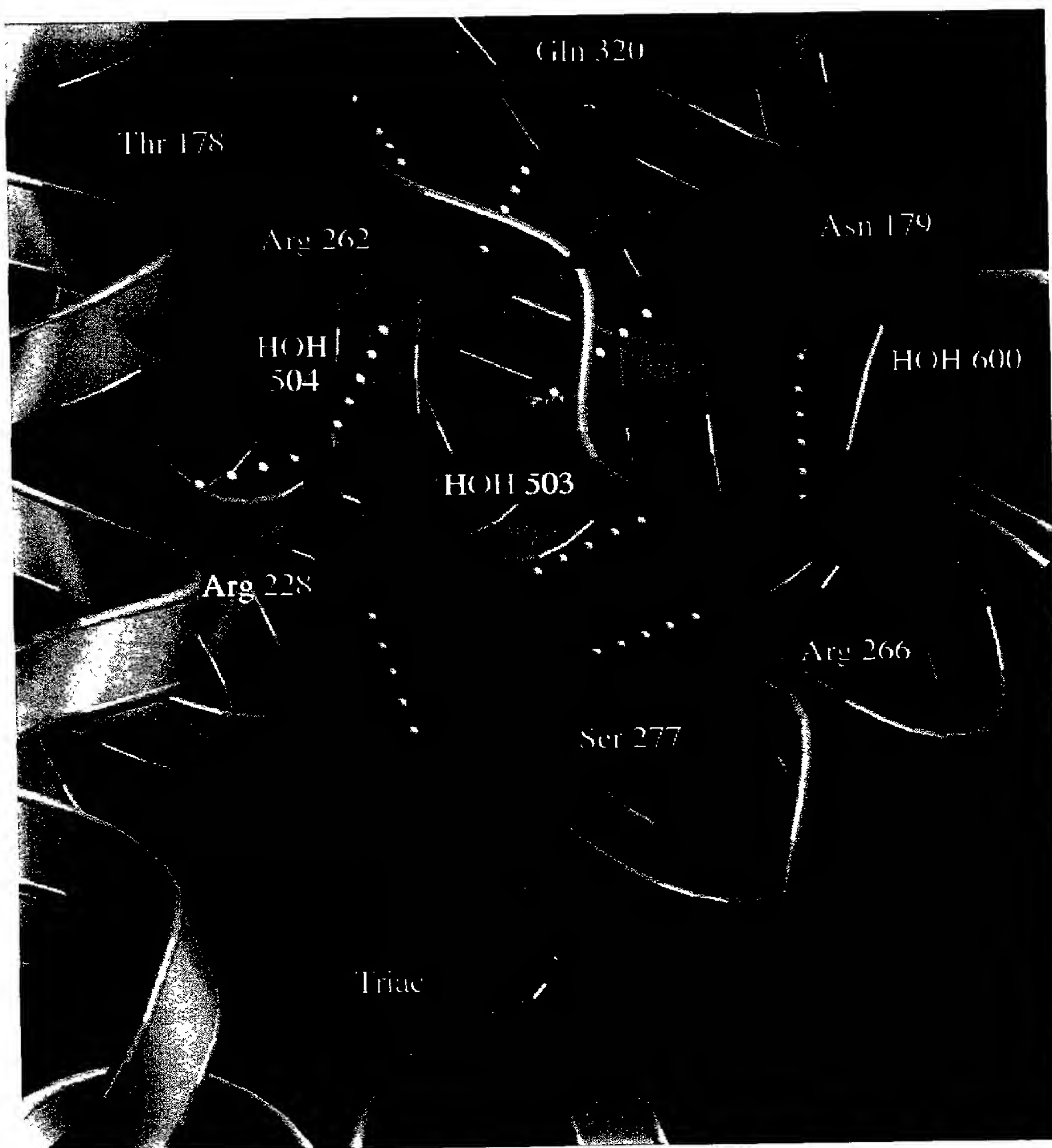




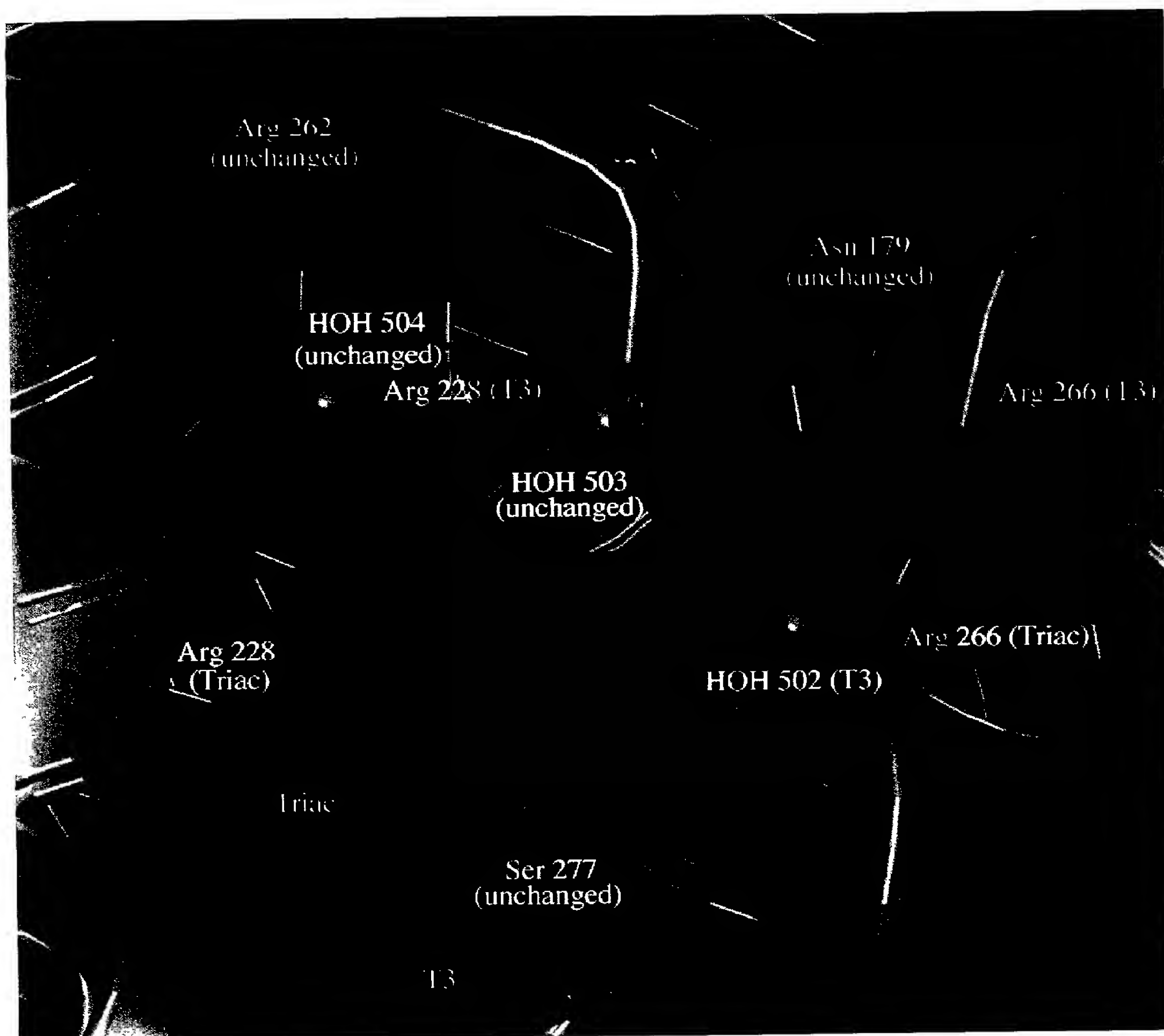
**FIG. 22**



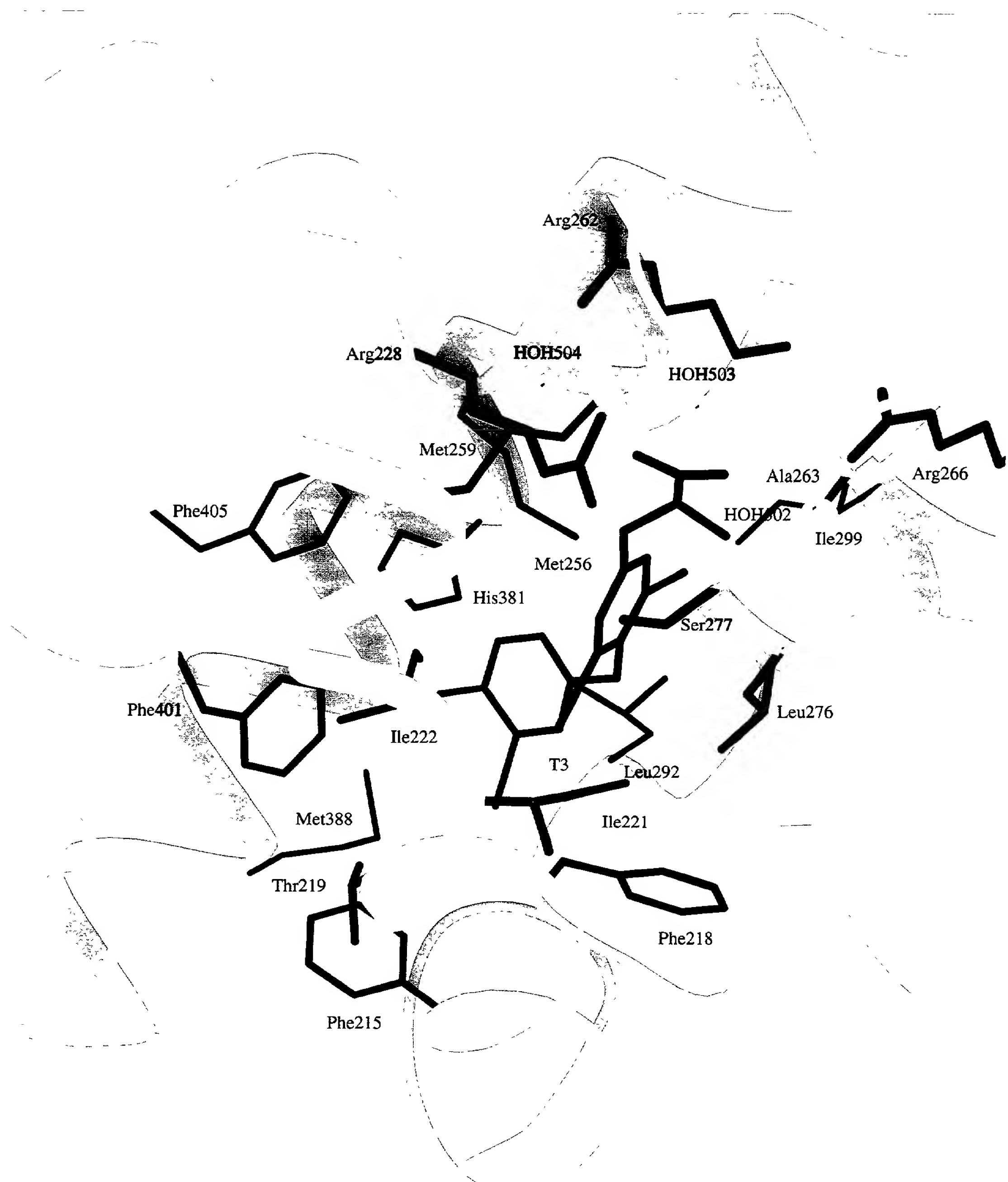
**FIG. 23**



**FIG. 24**

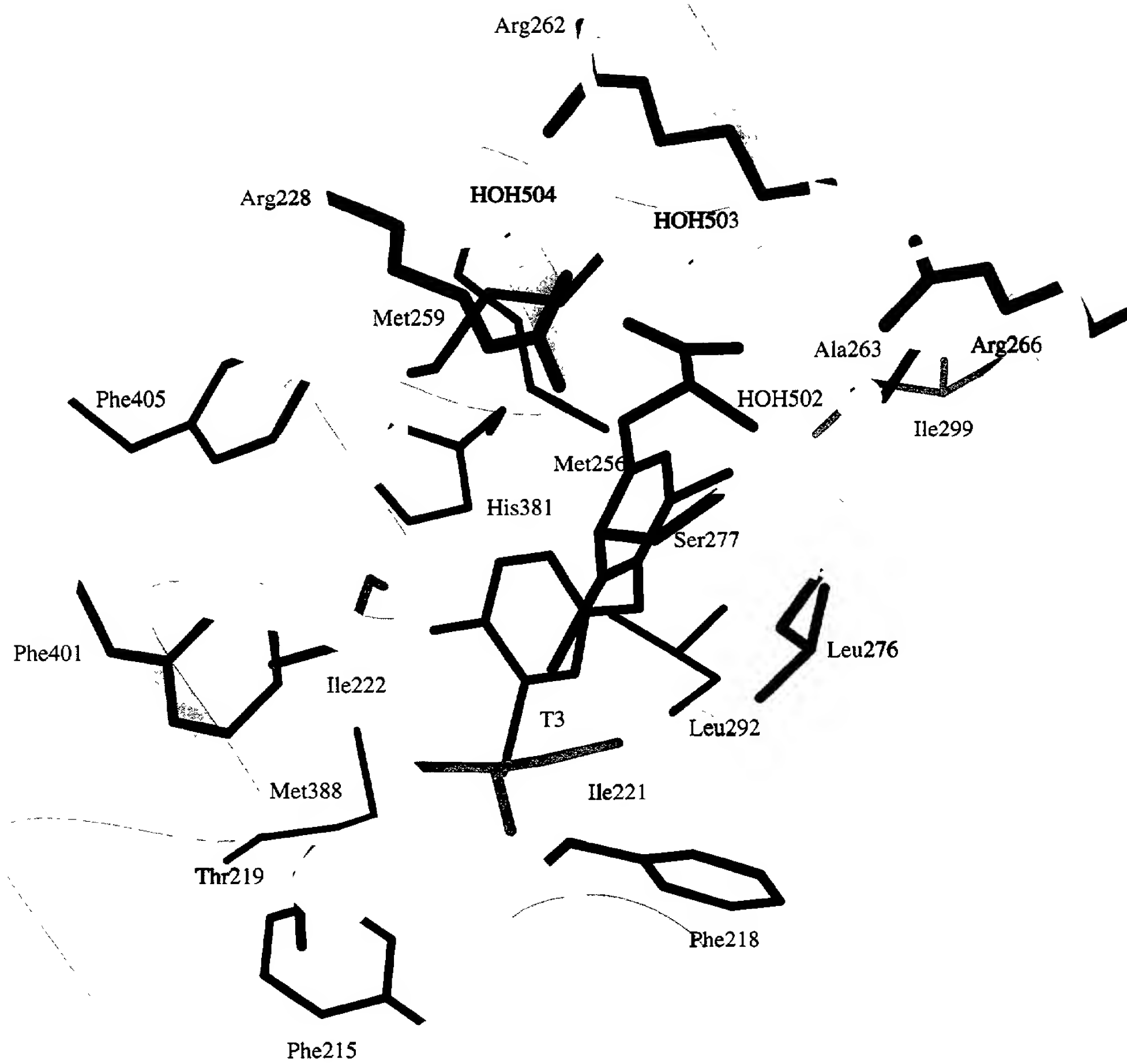


**FIG. 25**



**FIG. 26A**





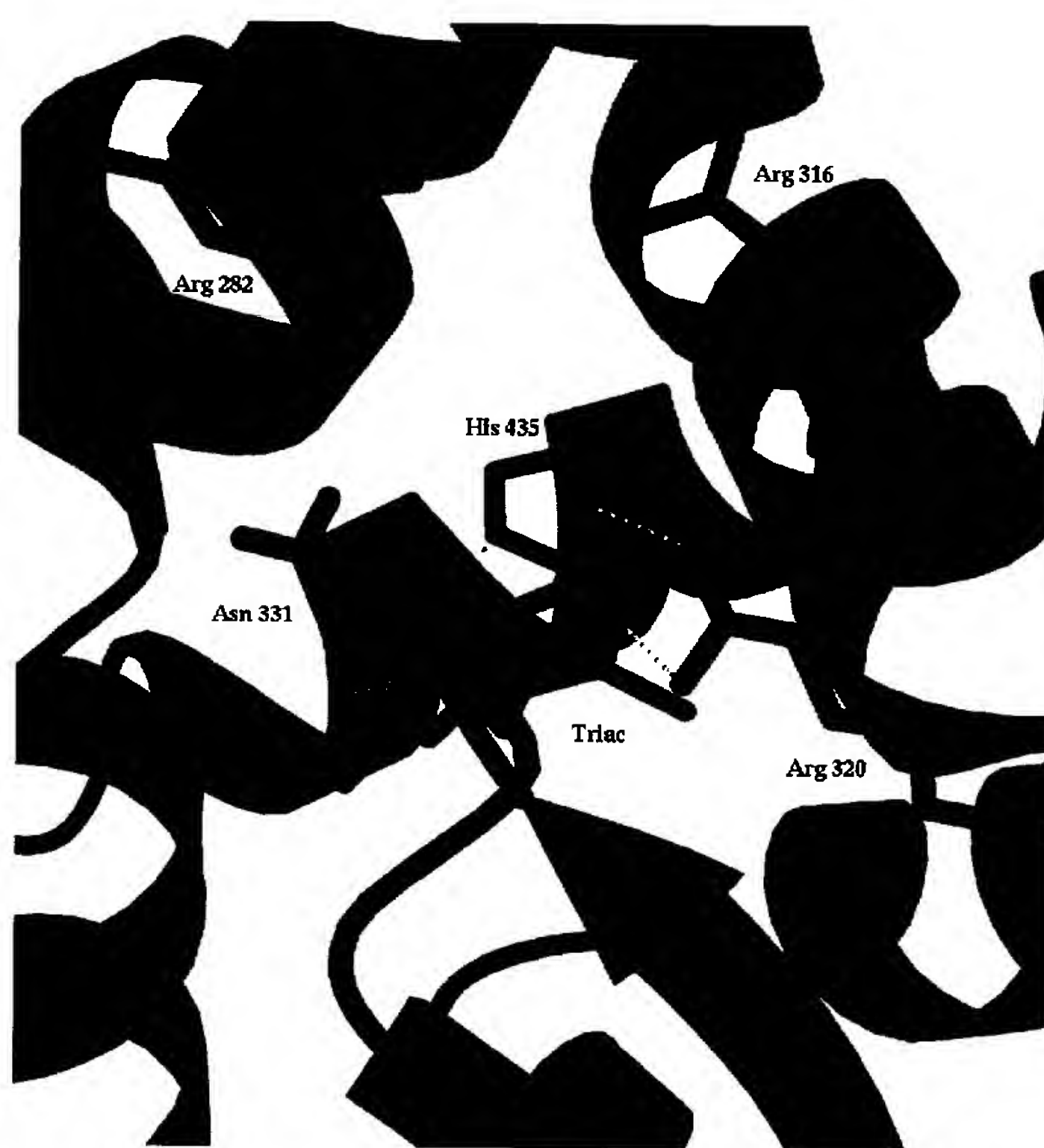
**FIG. 26B**

### Thyroid Hormone Receptor Beta with GC1



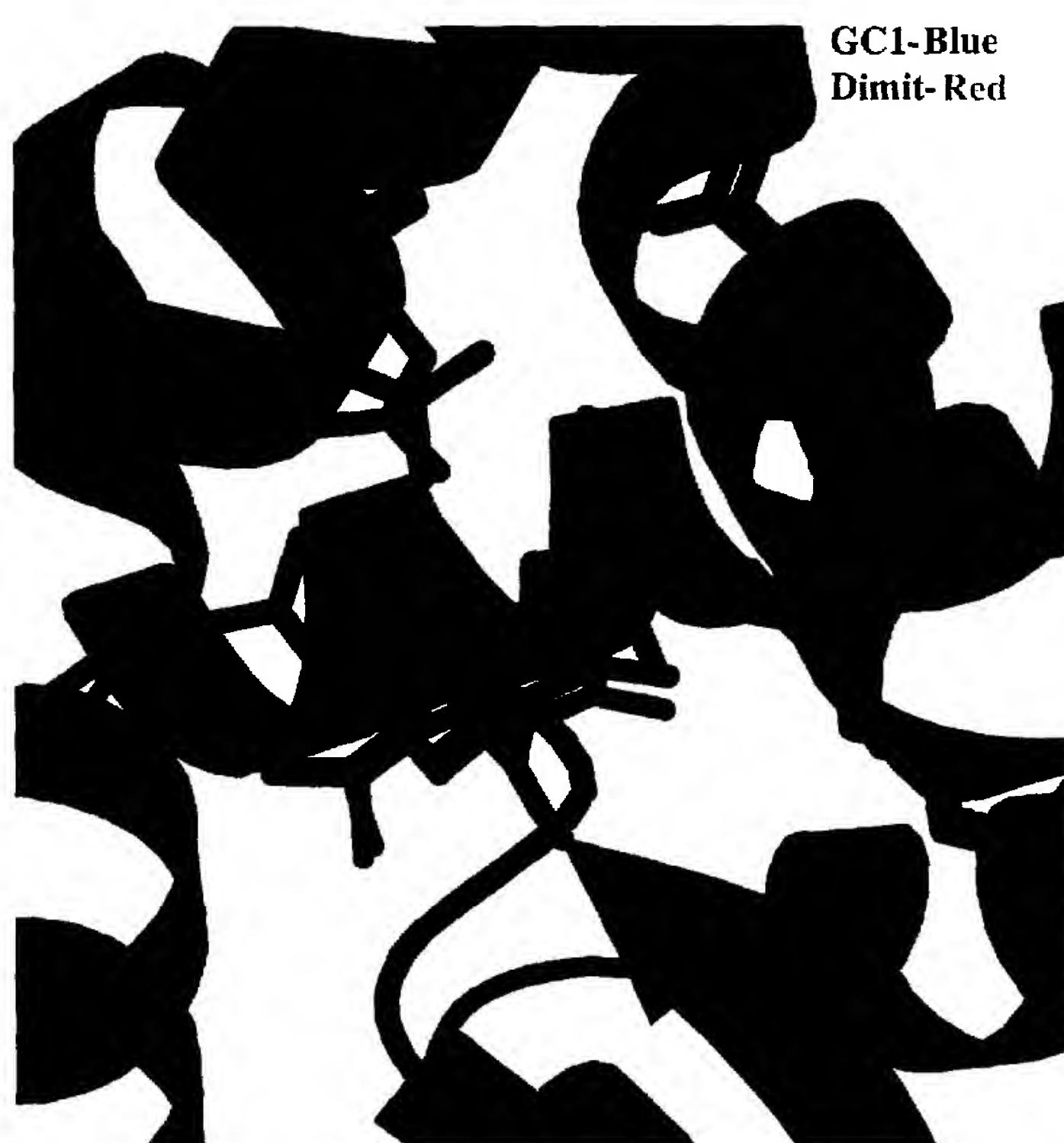
**FIG. 27**

Thyroid Hormone Receptor Beta with Triac



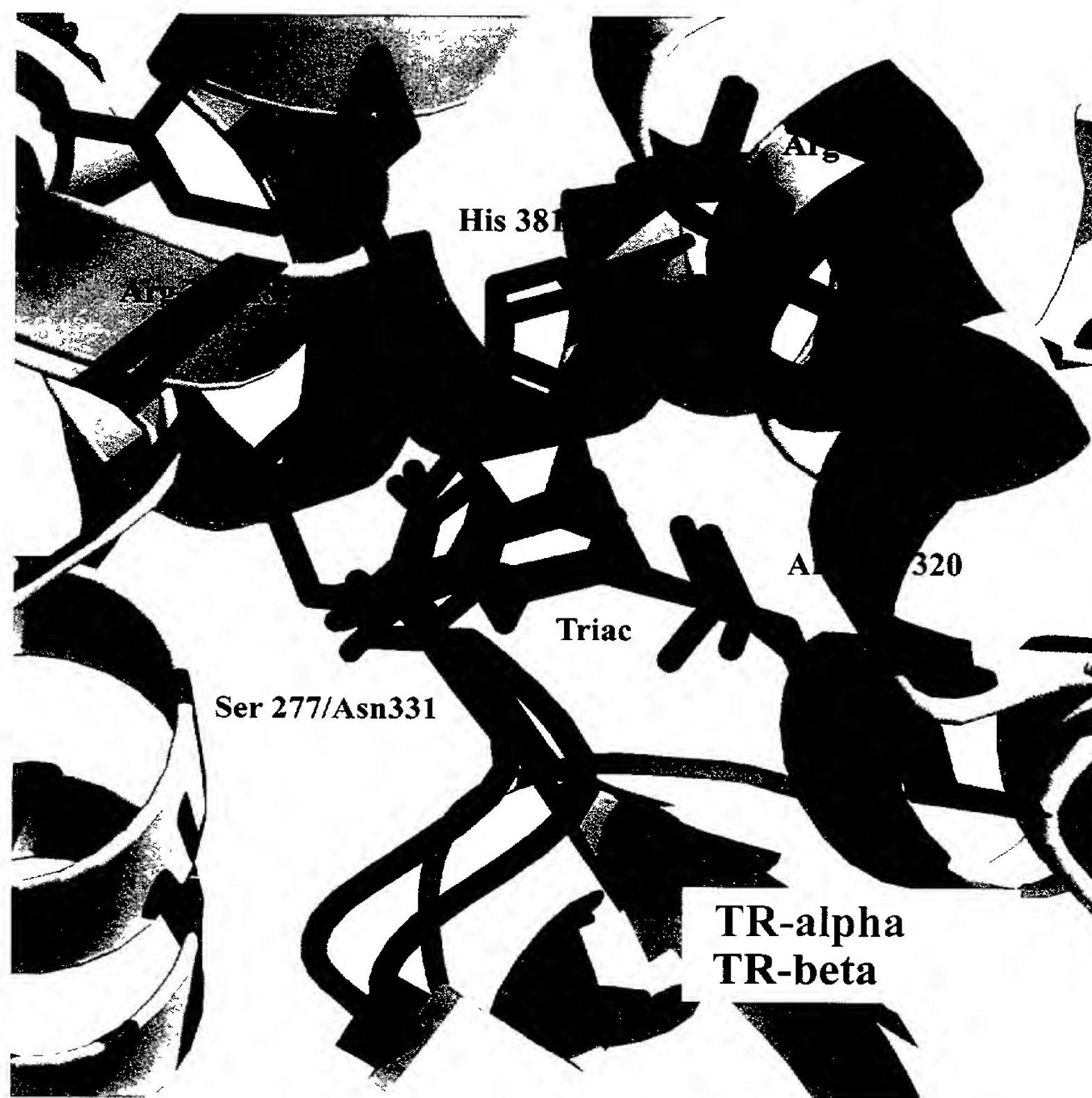
**FIG. 28**

**Structural Differences Between TR-b with GC1  
and TR-a with Dimit**



**FIG. 29**

**Structural Differences between TR LBD isoforms with Triac**

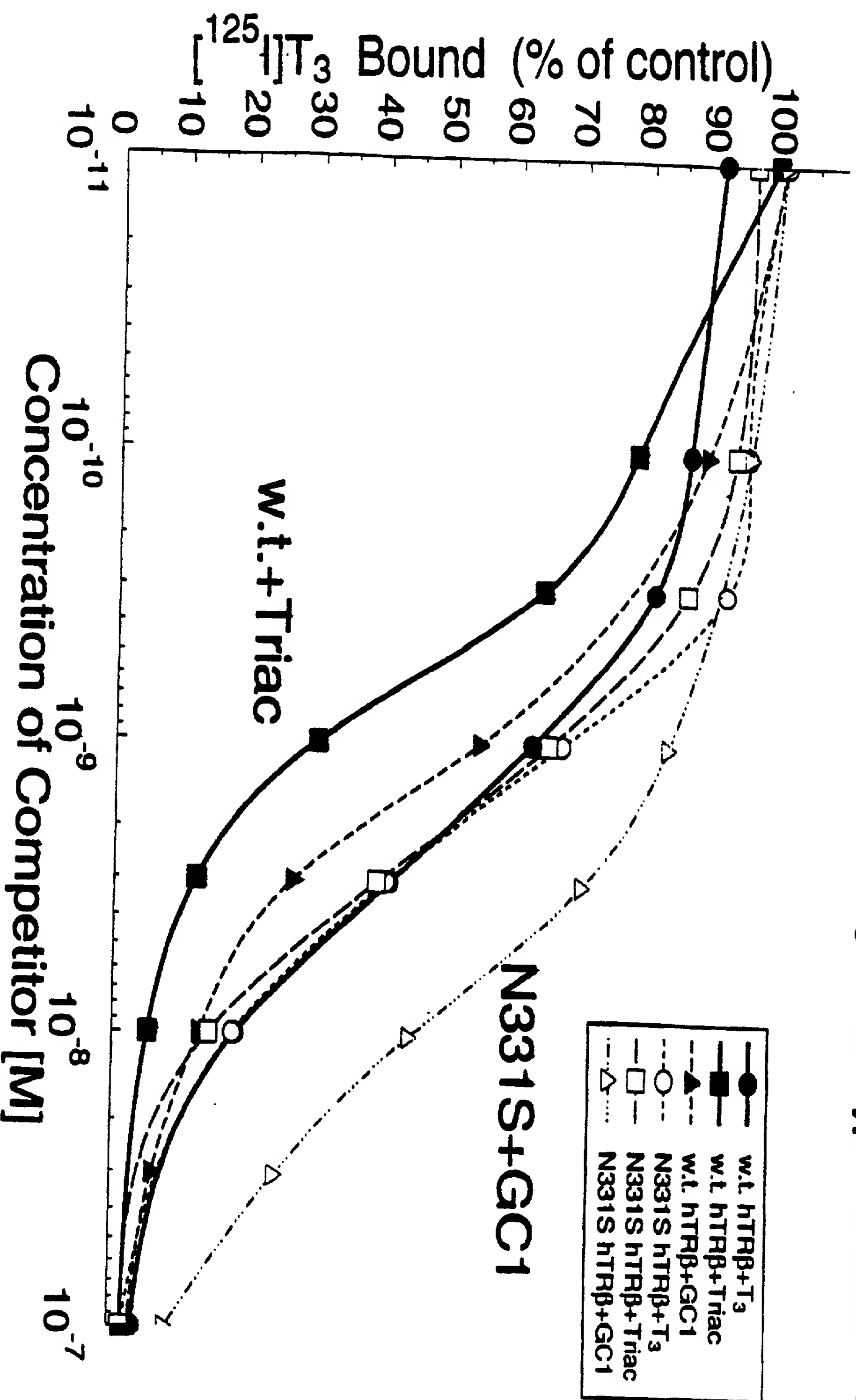


**FIG. 30**

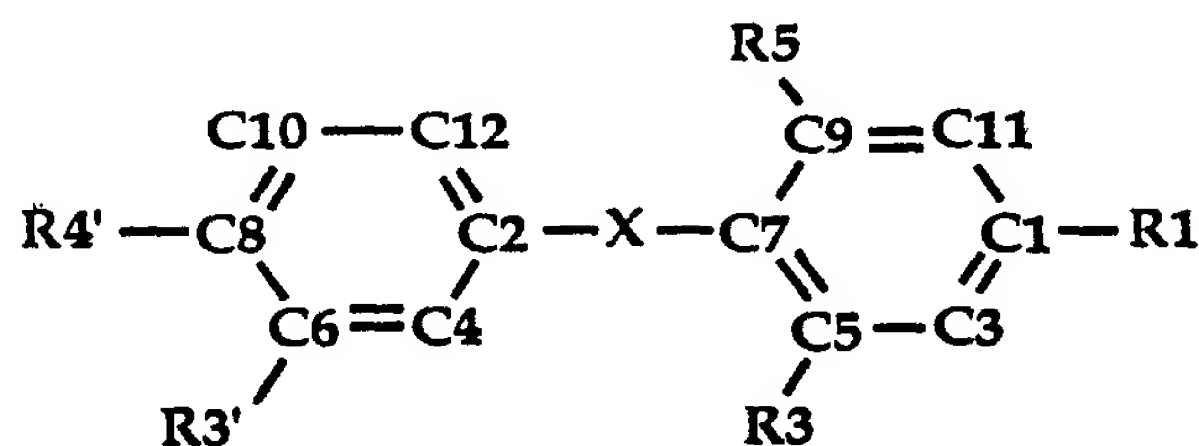


# FIG.31

Competition by T<sub>3</sub>, Triac & GC1 for [<sup>125</sup>I]T<sub>3</sub> binding to wild type and N331S hTRβ

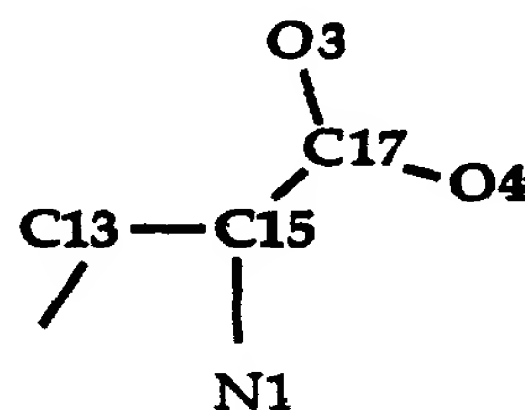


# Atomic Numbering for Thyronine-like Ligands

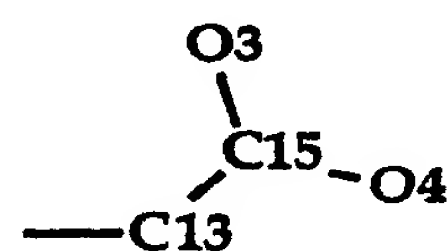


Ligand	R1	R3	R5	X	R3'	R4'
Dimit	amino propionic	C19	C20	O2	iPr	O1
IpBr <sub>2</sub>	amino propionic	BR1	BR2	O2	iPr	O1
T <sub>3</sub>	amino propionic	I1	I3	O2	I2	O1
Triac	acetic acid	I1	I3	O2	I2	O1
GC1	oxyacetic acid	C19	C20	C21	iPr	O1

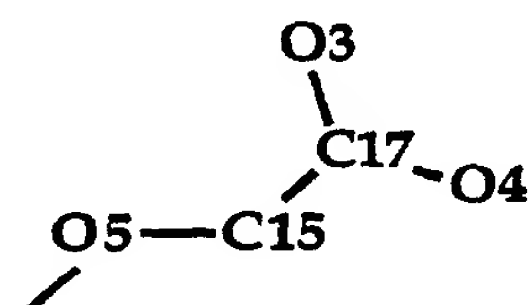
amino propionic acid



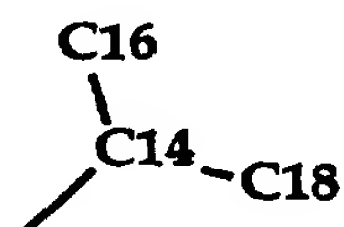
acetic acid



oxyacetic acid



isopropyl



**FIG.32**

DECLARATION AND POWER OF ATTORNEY

As a below named inventor, I hereby declare that:

My residence, post office address and citizenship are as stated next to my name.

I believe I am the original, first and sole inventor (if only one name is listed below) or an original, first and joint inventor (if plural names are listed below) of the subject matter which is claimed and for which a patent is sought on the invention entitled:

NUCLEAR RECEPTOR LIGANDS AND LIGAND BINDING DOMAINS

the specification of which:

☐ is attached hereto.

☒ was filed on November 26, 1997, and identified as Attorney Docket No. UCAL-246/02US.

☐ was filed on \_\_\_\_\_, as Application Serial No. \_\_\_\_\_.

and

☐ the amendment(s) of which were filed on \_\_\_\_\_.

I hereby state that I have reviewed and understand the contents of the above-identified specification, including the claims, as amended by any amendment referred to above.

I acknowledge the duty to disclose information which is material to the examination of this application in accordance with Title 37, Code of Federal Regulations, Section 1.56.

I hereby claim foreign priority benefits under title 35, United States Code, Section 119 of any foreign application(s) for patent or inventor's certificate listed below and have also identified below any foreign application for patent or inventor's certificate having a filing date before that of the application on which priority is claimed:

COPY

Prior Foreign Application(s) (Country) (Number) (Day/Month/Year Filed) Priority Claimed (Yes/No)

I hereby claim the benefit under Title 35, United States Code, § 119(e) of any United States provisional application(s) listed below.

<u>60/008,540</u> (Application Number)	<u>December 13, 1995</u> (Filing Date)
<u>60/008,543</u> (Application Number)	<u>December 13, 1995</u> (Filing Date)
<u>60/008,606</u> (Application Number)	<u>December 14, 1995</u> (Filing Date)

I hereby claim the benefit under Title 35, United States Code, Section 120 of any United States application(s) listed below and, insofar as the subject matter of each of the claims of this application is not disclosed in the prior United States application in the manner provided by the first paragraph of Title 35, United States Code, Section 112, I acknowledge the duty to disclose material information as defined in Title 37, Code of Federal Regulations, Section 1.56(a) which occurred between the filing date of the prior application and the national or PCT international filing date of this application:

<u>Appl. Ser. No.</u>	<u>Filing Date</u>	<u>Status (Pat'd./Pend./Aband.)</u>
08/764,870	December 13, 1996	Pending

I hereby appoint:

Jackie N. Nakamura	35,966	Richard L. Neeley	30,092
James A. Bradburne	38,389	David R. Stevens	38,626
Willis E. Higgins	23,025	Craig P. Opperman	37,078
Tom M. Moran	26,314	Melya J. Hughes	38,696
John W. Girvin, Jr.	22,706	Brian Lewis	32,502
Nina M. Ashton	37,273	Gurjeev K. Sachdeva	37,434
Marcella Lillis	36,583	Alexandra J. Baran	39,101
Peter R. Leal	24,226	Saul A. Seinberg	24,840

my attorneys and agents with full power of substitution and revocation to prosecute my above-identified application for Letters Patent and to transact all business in the Patent Office connected therewith.

I further direct that correspondence concerning this application be directed to

Attn: Jackie N. Nakamura  
COOLEY GODWARD LLP  
Five Palo Alto Square  
3000 El Camino Real  
Palo Alto, California 94306-2155  
Attention: Patent Group  
Telephone (650) 843-5000.

I hereby declare that all statements made herein of my own knowledge are true and that all statements made on information and belief are believed to be true; and further that these statements were made with the knowledge that willful false statements and the like so made are punishable by fine or imprisonment, or both, under Section 1001 of Title 18 of the United States Code and that such willful false statements may jeopardize the validity of the application or any patent issued thereon.

Full name of first inventor: Thomas S. Scanlan

Inventor's signature

*Thomas S. Scanlan*

Date

*3/6/98*

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San Francisco, California 94122

Citizen of:

U.S.A.

Post Office Address:

Same

Full name of second inventor: John D. Baxter

Inventor's signature

*John D. Baxter*

Date

*3/30/98*

Residence:

131 San Pablo Avenue  
San Francisco, California 94127

Citizen of:

U.S.A.

Post Office Address:

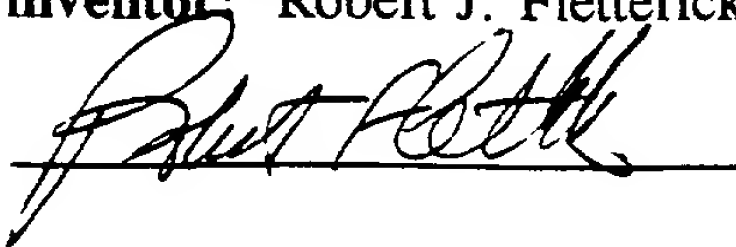
Same

COPY



**Full name of third inventor:** Robert J. Fletterick

Inventor's signature



Date

3/6/98

Residence:

15 Christopher Avenue  
San Francisco, California 94131

Citizen of:

U.S.A.

Post Office Address:

Same

**Full name of fourth inventor:** Richard L. Wagner

Inventor's signature



Date

3/20/98

Residence:

1701 Waller Street  
San Francisco, California 94117

Citizen of:

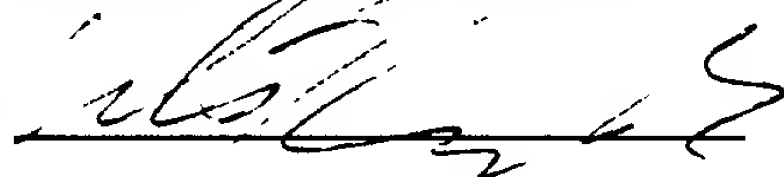
U.S.A.

Post Office Address:

Same

**Full name of fifth inventor:** Peter J. Kushner

Inventor's signature



Date

3/27/98

Residence:

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Citizen of:

U.S.A.

Post Office Address:

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Full name of sixth inventor: James <sup>W. JWH</sup> Apriletti

Inventor's signature

James W. Apriletti

Date

3-27-98

Residence:

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Berkeley, California 94702

Citizen of:

U.S.A.

Post Office Address:

Same

Full name of seventh inventor: Brian <sup>L. B.L.W</sup> West

Inventor's signature

Brian L. West

Date

March 27, 1998

Residence:

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Citizen of:

U.S.A.

Post Office Address:

Same

Full name of Eighth inventor: Andrew K. Shiau

Inventor's signature

Andrew K. Shiau

Date

03/20/98

Residence:

34 Hugo Street, #3  
San Francisco, California 94122

Citizen of:

U.S.A.

Post Office Address:

Same

COPY

# SEQUENCE LISTING

<110> Baxter, John  
Fletterick, Robert  
Kushner, Peter

<120> NUCLEAR RECEPTOR LIGANDS AND LIGAND BINDING DOMAINS

<130> UCAL-246/02/1US

<140> Not Yet Available

<141> 2000-08-10

<150> US 08/980,115

<151> 1997-11-26

<150> US 08/764,870

<151> 1996-12-13

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<222> (157)..(410)

<223> minimal ligand binding domain

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<222> (393)..(405)

<223> activation domain

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Asn Ser Ala Arg Ser Pro Asp Gly Lys Arg Lys Arg Lys Asn Gly Gln  
20 25 30



Lys Ile Glu Lys Ser Gln Glu Ala Tyr Leu Leu Ala Phe Glu His Tyr  
 340 345 350

Val Asn His Arg Lys His Asn Ile Pro His Phe Trp Pro Lys Leu Leu  
 355 360 365

Met Lys Val Thr Asp Leu Arg Met Ile Gly Ala Cys His Ala Ser Arg  
 370 375 380

Phe Leu His Met Lys Val Glu Cys Pro Thr Glu Leu Phe Pro Pro Leu  
 385 390 395 400

Phe Leu Glu Val Phe Glu Asp Gln Glu Val  
 405 410

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 <223> minimal ligand binding domain

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Met Glu Gln Lys Pro Ser Lys Val Glu Cys Gly Ser Asp Pro Glu Glu  
 1 5 10 15

Asn Ser Ala Arg Ser Pro Asp Gly Lys Arg Lys Arg Lys Asn Gly Gln  
 20 25 30

Cys Ser Leu Lys Thr Ser Met Ser Gly Tyr Ile Pro Ser Tyr Leu Asp  
 35 40 45

Lys Asp Glu Gln Cys Val Val Cys Gly Asp Lys Ala Thr Gly Tyr His  
 50 55 60

Tyr Arg Cys Ile Thr Cys Glu Gly Cys Lys Gly Phe Phe Arg Arg Thr  
 65 70 75 80

Ile Gln Lys Asn Leu His Pro Thr Tyr Ser Cys Lys Tyr Asp Ser Cys  
 85 90 95

Cys Val Ile Asp Lys Ile Thr Arg Asn Gln Cys Gln Leu Cys Arg Phe  
 100 105 110

Lys Lys Cys Ile Ala Val Gly Met Ala Met Asp Leu Val Leu Asp Asp  
 115 120 125

Ser Lys Arg Val Ala Lys Arg Lys Leu Ile Glu Gln Asn Arg Glu Arg  
 130 135 140

Arg Arg Lys Glu Glu Met Ile Arg Ser Leu Gln Gln Arg Pro Glu Pro  
 145 150 155 160



Thr	Pro	Glu	Glu	Trp	Asp	Leu	Ile	His	Ile	Ala	Thr	Glu	Ala	His	Arg	
				165					170					175		
Ser	Thr	Asn	Ala	Gln	Gly	Ser	His	Trp	Lys	Gln	Arg	Arg	Lys	Phe	Leu	
			180					185					190			
Pro	Asp	Asp	Ile	Gly	Gln	Ser	Pro	Ile	Val	Ser	Met	Pro	Asp	Gly	Asp	
		195					200					205				
Lys	Val	Asp	Leu	Glu	Ala	Phe	Ser	Glu	Phe	Thr	Lys	Ile	Ile	Thr	Pro	
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Ala	Ile	Thr	Arg	Val	Val	Asp	Phe	Ala	Lys	Lys	Leu	Pro	Met	Phe	Ser	
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Glu	Leu	Pro	Cys	Glu	Asp	Gln	Ile	Ile	Leu	Leu	Lys	Gly	Cys	Cys	Met	
			245					250						255		
Glu	Ile	Met	Ser	Leu	Arg	Ala	Ala	Val	Arg	Tyr	Asp	Pro	Glu	Ser	Asp	
		260						265					270			
Thr	Leu	Thr	Leu	Ser	Gly	Glu	Met	Ala	Val	Lys	Arg	Glu	Gln	Leu	Lys	
		275					280					285				
Asn	Gly	Gly	Leu	Gly	Val	Val	Ser	Asp	Ala	Ile	Phe	Glu	Leu	Gly	Lys	
	290					295					300					
Ser	Leu	Ser	Ala	Phe	Asn	Leu	Asp	Asp	Thr	Glu	Val	Ala	Leu	Leu	Gln	
305					310					315					320	
Ala	Val	Leu	Leu	Met	Ser	Thr	Asp	Arg	Ser	Gly	Leu	Leu	Cys	Val	Asp	
				325					330					335		
Lys	Ile	Glu	Lys	Ser	Gln	Glu	Ala	Tyr	Leu	Leu	Ala	Phe	Glu	His	Tyr	
			340					345					350			
Val	Asn	His	Arg	Lys	His	Asn	Ile	Pro	His	Phe	Trp	Pro	Lys	Leu	Leu	
		355					360					365				
Met	Lys	Val	Thr	Asp	Leu	Arg	Met	Ile	Gly	Ala	Cys	His	Ala	Ser	Arg	
	370					375					380					
Phe	Leu	His	Met	Lys	Val	Glu	Cys	Pro	Thr	Glu	Leu	Phe	Pro	Pro	Leu	
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Phe	Leu	Glu	Val	Phe	Glu	Asp	Gln	Glu	Val							
				405				410								

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<223> minimal ligand binding domain

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Met Thr Pro Asn Ser Met Thr Glu Asn Gly Leu Thr Ala Trp Asp Lys  
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Pro Lys His Cys Pro Asp Arg Glu His Asp Trp Lys Leu Val Gly Met  
20 25 30  
Ser Glu Ala Cys Leu His Arg Lys Ser His Ser Glu Arg Arg Ser Thr  
35 40 45  
Leu Lys Asn Glu Gln Ser Ser Pro His Leu Ile Gln Thr Thr Trp Thr  
50 55 60  
Ser Ser Ile Phe His Leu Asp His Asp Asp Val Asn Asp Gln Ser Val  
65 70 75 80  
Ser Ser Ala Gln Thr Phe Gln Thr Glu Glu Lys Lys Cys Lys Gly Tyr  
85 90 95  
Ile Pro Ser Tyr Leu Asp Lys Asp Glu Leu Cys Val Val Cys Gly Asp  
100 105 110  
Lys Ala Thr Gly Tyr His Tyr Arg Cys Ile Thr Cys Glu Gly Cys Lys  
115 120 125  
Gly Phe Phe Arg Arg Thr Ile Gln Lys Asn Leu His Pro Ser Tyr Ser  
130 135 140  
Cys Lys Tyr Glu Gly Lys Cys Val Ile Asp Lys Val Thr Arg Asn Gln  
145 150 155 160  
Cys Gln Glu Cys Arg Phe Lys Lys Cys Ile Tyr Val Gly Met Ala Thr  
165 170 175  
Asp Leu Val Leu Asp Asp Ser Lys Arg Leu Ala Lys Arg Lys Leu Ile  
180 185 190  
Glu Glu Asn Arg Glu Lys Arg Arg Arg Glu Glu Leu Gln Lys Ser Ile  
195 200 205  
Gly His Lys Pro Glu Pro Thr Asp Glu Glu Trp Glu Leu Ile Lys Thr  
210 215 220  
Val Thr Glu Ala His Val Ala Thr Asn Ala Gln Gly Ser His Trp Lys  
225 230 235 240  
Gln Lys Pro Lys Phe Leu Pro Glu Asp Ile Gly Gln Ala Pro Ile Val  
245 250 255  
Asn Ala Pro Glu Gly Gly Lys Val Asp Leu Glu Ala Phe Ser His Phe  
260 265 270  
Thr Lys Ile Ile Thr Pro Ala Ile Thr Arg Val Val Asp Phe Ala Lys

275		280		285
Lys Leu Pro Met Phe Cys Glu Leu Pro Cys Glu Asp Gln Ile Ile Leu				
290		295		300
Leu Lys Gly Cys Cys Met Glu Ile Met Ser Leu Arg Ala Ala Val Arg				
305		310		315 320
Tyr Asp Pro Glu Ser Glu Thr Leu Thr Leu Asn Gly Glu Met Ala Val				
	325		330	335
Ile Arg Gly Gln Leu Lys Asn Gly Gly Leu Gly Val Val Ser Asp Ala				
	340		345	350
Ile Phe Asp Leu Gly Met Ser Leu Ser Ser Phe Asn Leu Asp Asp Thr				
	355		360	365
Glu Val Ala Leu Leu Gln Ala Val Leu Leu Met Ser Ser Asp Arg Pro				
	370		375	380
Gly Leu Ala Cys Val Glu Arg Ile Glu Lys Tyr Gln Asp Ser Phe Leu				
385		390		395 400
Leu Ala Phe Glu His Tyr Ile Asn Tyr Arg Lys His His Val Thr His				
	405		410	415
Phe Trp Pro Lys Leu Leu Met Lys Val Thr Asp Leu Arg Met Ile Gly				
	420		425	430
Ala Cys His Ala Ser Arg Phe Leu His Met Lys Val Glu Cys Pro Thr				
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	450		455	460

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 <211> 416  
 <212> PRT  
 <213> Homo sapiens

<220>  
 <221> DOMAIN  
 <222> (131)..(373)  
 <223> minimal ligand binding domain

<400> 4

Pro Asn Ser Asn His Val Ala Ser Gly Ala Gly Glu Ala Ala Ile Glu				
1	5		10	15
Thr Gln Ser Ser Ser Ser Glu Glu Ile Val Pro Ser Pro Pro Ser Pro				
	20		25	30
Pro Pro Leu Pro Arg Ile Tyr Lys Pro Cys Phe Val Cys Gln Asp Lys				
	35		40	45



Lys Met Glu Ile Pro Gly Ser Met Pro Pro Leu Ile Gln Glu Met Leu  
 355 360 365

Glu Asn Ser Glu Gly Leu Asp Thr Leu Ser Gly Gln Pro Gly Gly Gly  
 370 375 380

Gly Arg Asp Gly Gly Gly Leu Ala Pro Pro Pro Gly Ser Cys Ser Pro  
 385 390 395 400

Ser Leu Ser Pro Ser Ser Asn Arg Ser Ser Pro Ala Thr His Ser Pro  
 405 410 415

<210> 5

<211> 454

<212> PRT

<213> Homo sapiens

<220>

<221> DOMAIN

<222> (179)..(421)

<223> minimal ligand binding domain

<400> 5

Met Ala Thr Asn Lys Glu Arg Leu Phe Ala Ala Gly Ala Leu Gly Pro  
 1 5 10 15

Gly Ser Gly Tyr Pro Gly Ala Gly Phe Pro Phe Ala Phe Pro Gly Ala  
 20 25 30

Leu Arg Gly Ser Pro Pro Phe Glu Met Leu Ser Pro Ser Phe Arg Gly  
 35 40 45

Leu Gly Gln Pro Asp Leu Pro Lys Glu Met Ala Ser Leu Ser Val Glu  
 50 55 60

Thr Gln Ser Thr Ser Ser Glu Glu Met Val Pro Ser Ser Pro Ser Pro  
 65 70 75 80

Pro Pro Pro Pro Arg Val Tyr Lys Pro Cys Phe Val Cys Asn Asp Lys  
 85 90 95

Ser Ser Gly Tyr His Tyr Gly Val Ser Ser Cys Glu Gly Cys Lys Gly  
 100 105 110

Phe Phe Arg Arg Ser Ile Gln Lys Asn Met Val Tyr Thr Cys His Arg  
 115 120 125

Asp Lys Asn Cys Ile Ile Asn Lys Val Thr Arg Asn Arg Cys Gln Tyr  
 130 135 140

Cys Arg Leu Gln Lys Cys Phe Glu Val Gly Met Ser Lys Glu Ala Val  
 145 150 155 160

Arg Asn Asp Arg Asn Lys Lys Lys Lys Glu Val Lys Glu Glu Gly Ser  
 165 170 175





<212> PRT  
 <213> Homo sapiens

<220>  
 <221> DOMAIN  
 <222> (231)..(460)  
 <223> minimal ligand binding domain

<400> 6

Met	Asp	Thr	Lys	His	Phe	Leu	Pro	Leu	Asp	Phe	Ser	Thr	Gln	Val	Asn			
1				5					10					15				
Ser	Ser	Leu	Thr	Ser	Pro	Thr	Gly	Arg	Gly	Ser	Met	Ala	Ala	Pro	Ser			
			20					25					30					
Leu	His	Pro	Ser	Leu	Gly	Pro	Gly	Ile	Gly	Ser	Pro	Gly	Gln	Leu	His			
			35				40					45						
Ser	Pro	Ile	Ser	Thr	Leu	Ser	Ser	Pro	Ile	Asn	Gly	Met	Gly	Pro	Pro			
	50					55					60							
Phe	Ser	Val	Ile	Ser	Ser	Pro	Met	Gly	Pro	His	Ser	Met	Ser	Val	Pro			
65					70					75					80			
Thr	Thr	Pro	Thr	Leu	Gly	Phe	Ser	Thr	Gly	Ser	Pro	Gln	Leu	Ser	Ser			
				85					90					95				
Pro	Met	Asn	Pro	Val	Ser	Ser	Ser	Glu	Asp	Ile	Lys	Pro	Pro	Leu	Gly			
			100					105					110					
Leu	Asn	Gly	Val	Leu	Lys	Val	Pro	Ala	His	Pro	Ser	Gly	Asn	Met	Ala			
		115					120					125						
Ser	Phe	Thr	Lys	His	Ile	Cys	Ala	Ile	Cys	Gly	Asp	Arg	Ser	Ser	Gly			
	130					135					140							
Lys	His	Tyr	Gly	Val	Tyr	Ser	Cys	Glu	Gly	Cys	Lys	Gly	Phe	Phe	Lys			
145					150					155					160			
Arg	Thr	Val	Arg	Lys	Asp	Leu	Thr	Tyr	Thr	Cys	Arg	Asp	Asn	Lys	Asp			
				165					170					175				
Cys	Leu	Ile	Asp	Lys	Arg	Gln	Arg	Asn	Arg	Cys	Gln	Tyr	Cys	Arg	Tyr			
			180					185					190					
Gln	Lys	Cys	Leu	Ala	Met	Gly	Met	Lys	Arg	Glu	Ala	Val	Gln	Glu	Glu			
		195					200					205						
Arg	Gln	Arg	Gly	Lys	Asp	Arg	Asn	Glu	Asn	Glu	Val	Glu	Ser	Thr	Ser			
	210					215					220							
Ser	Ala	Asn	Glu	Asp	Met	Pro	Val	Glu	Arg	Ile	Leu	Glu	Ala	Glu	Leu			
225					230					235					240			
Ala	Val	Glu	Pro	Lys	Thr	Glu	Thr	Tyr	Val	Glu	Ala	Asn	Met	Gly	Leu			

245										250					255				
Asn	Pro	Ser	Ser	Pro	Asn	Asp	Pro	Val	Thr	Asn	Ile	Cys	Gln	Ala	Ala				
			260					265					270						
Asp	Lys	Gln	Leu	Phe	Thr	Leu	Val	Glu	Trp	Ala	Lys	Arg	Ile	Pro	His				
		275					280					285							
Phe	Ser	Glu	Leu	Pro	Leu	Asp	Asp	Gln	Val	Ile	Leu	Leu	Arg	Ala	Gly				
	290					295					300								
Trp	Asn	Glu	Leu	Leu	Ile	Ala	Ser	Phe	Ser	His	Arg	Ser	Ile	Ala	Val				
305					310					315					320				
Lys	Asp	Gly	Ile	Leu	Leu	Ala	Thr	Gly	Leu	His	Val	His	Arg	Asn	Ser				
			325						330					335					
Ala	His	Ser	Ala	Gly	Val	Gly	Ala	Ile	Phe	Asp	Arg	Val	Leu	Thr	Glu				
			340					345					350						
Leu	Val	Ser	Lys	Met	Arg	Asp	Met	Gln	Met	Asp	Lys	Thr	Glu	Leu	Gly				
		355					360					365							
Cys	Leu	Arg	Ala	Ile	Val	Leu	Phe	Asn	Pro	Asp	Ser	Lys	Gly	Leu	Ser				
	370					375					380								
Asn	Pro	Ala	Glu	Val	Glu	Ala	Leu	Arg	Glu	Lys	Val	Tyr	Ala	Ser	Leu				
385					390					395					400				
Glu	Ala	Tyr	Cys	Lys	His	Lys	Tyr	Pro	Glu	Gln	Pro	Gly	Arg	Phe	Ala				
				405					410					415					
Lys	Leu	Leu	Leu	Arg	Leu	Pro	Ala	Leu	Arg	Ser	Ile	Gly	Leu	Lys	Cys				
			420					425					430						
Leu	Glu	His	Leu	Phe	Phe	Phe	Lys	Leu	Ile	Gly	Asp	Thr	Pro	Ile	Asp				
		435					440					445							
Thr	Phe	Leu	Met	Glu	Met	Leu	Glu	Ala	Pro	His	Gln	Met	Thr						
	450					455					460								

<210> 7  
 <211> 525  
 <212> PRT  
 <213> Homo sapiens

<220>  
 <221> DOMAIN  
 <222> (292)..(523)  
 <223> minimal ligand binding domain

<400> 7

Met	Ser	Trp	Ala	Ala	Arg	Pro	Pro	Phe	Leu	Pro	Gln	Arg	His	Ala	Glu	
1				5					10					15		



Gly Ser Ser Pro Asn Asp Pro Val Thr Asn Ile Cys Gln Ala Ala Asp  
 325 330 335  
 Lys Gln Leu Phe Thr Leu Val Glu Trp Ala Lys Arg Ile Pro His Phe  
 340 345 350  
 Ser Ser Leu Pro Leu Asp Asp Gln Val Ile Leu Leu Arg Ala Gly Trp  
 355 360 365  
 Asn Glu Leu Leu Ile Ala Ser Phe Ser His Arg Ser Ile Asp Val Arg  
 370 375 380  
 Asp Gly Ile Leu Leu Ala Thr Gly Leu His Val His Arg Asn Ser Ala  
 385 390 395 400  
 His Ser Ala Gly Val Gly Ala Ile Phe Asp Arg Val Leu Thr Glu Leu  
 405 410 415  
 Val Ser Lys Met Arg Asp Met Arg Met Asp Lys Thr Glu Leu Gly Cys  
 420 425 430  
 Leu Arg Ala Ile Ile Leu Phe Asn Pro Asp Ala Lys Gly Leu Ser Asn  
 435 440 445  
 Pro Ser Glu Val Glu Val Leu Arg Glu Lys Val Tyr Ala Ser Leu Glu  
 450 455 460  
 Thr Tyr Cys Lys Gln Lys Tyr Pro Glu Gln Gln Gly Arg Phe Ala Lys  
 465 470 475 480  
 Leu Leu Leu Arg Leu Pro Ala Leu Arg Ser Ile Gly Leu Lys Cys Leu  
 485 490 495  
 Glu His Leu Phe Phe Phe Lys Leu Ile Gly Asp Thr Pro Ile Asp Thr  
 500 505 510  
 Phe Leu Met Glu Met Leu Glu Ala Pro His Gln Leu Ala  
 515 520 525

<210> 8  
 <211> 468  
 <212> PRT  
 <213> Homo sapiens

<220>  
 <221> DOMAIN  
 <222> (196)..(468)  
 <223> minimal ligand binding domain

<400> 8

Met Val Asp Thr Glu Ser Pro Leu Cys Pro Leu Ser Pro Leu Glu Ala  
 1 5 10 15  
 Gly Asp Leu Glu Ser Pro Leu Ser Glu Glu Phe Leu Gln Glu Met Gly  
 20 25 30





Gly Phe Ile Thr Arg Glu Phe Leu Lys Ser Leu Arg Lys Pro Phe Cys  
 340 345 350  
 Asp Ile Met Glu Pro Lys Phe Asp Phe Ala Met Lys Phe Asn Ala Leu  
 355 360 365  
 Glu Leu Asp Asp Ser Asp Ile Ser Leu Phe Val Ala Ala Ile Ile Cys  
 370 375 380  
 Cys Gly Asp Arg Pro Gly Leu Leu Asn Val Gly His Ile Glu Lys Met  
 385 390 395 400  
 Gln Glu Gly Ile Val His Val Leu Arg Leu His Leu Gln Ser Asn His  
 405 410 415  
 Pro Asp Asp Ile Phe Leu Phe Pro Lys Leu Leu Gln Lys Met Ala Asp  
 420 425 430  
 Leu Arg Gln Leu Val Thr Glu His Ala Gln Leu Val Gln Ile Ile Lys  
 435 440 445  
 Lys Thr Glu Ser Asp Ala Ala Leu His Pro Leu Leu Gln Glu Ile Tyr  
 450 455 460

Arg Asp Met Tyr  
 465

<210> 9  
 <211> 441  
 <212> PRT  
 <213> Homo sapiens  
  
 <220>  
 <221> DOMAIN  
 <222> (168)..(441)  
 <223> minimal ligand binding domain

<400> 9

Met Glu Gln Pro Gln Glu Glu Ala Pro Glu Val Arg Glu Glu Glu Glu  
 1 5 10 15  
 Lys Glu Glu Val Ala Glu Ala Glu Gly Ala Pro Glu Leu Asn Gly Gly  
 20 25 30  
 Pro Gln His Ala Leu Pro Ser Ser Ser Tyr Thr Asp Leu Ser Arg Ser  
 35 40 45  
 Ser Ser Pro Pro Ser Leu Leu Asp Gln Leu Gln Met Gly Cys Asp Gly  
 50 55 60  
 Ala Ser Cys Gly Ser Leu Asn Met Glu Cys Arg Val Cys Gly Asp Lys  
 65 70 75 80  
 Ala Ser Gly Phe His Tyr Gly Val His Ala Cys Glu Gly Cys Lys Gly

85								90				95			
Phe	Phe	Arg	Arg	Thr	Ile	Arg	Met	Lys	Leu	Glu	Tyr	Glu	Lys	Cys	Glu
			100					105					110		
Arg	Ser	Cys	Lys	Ile	Gln	Lys	Lys	Asn	Arg	Asn	Lys	Cys	Gln	Tyr	Cys
		115					120					125			
Arg	Phe	Gln	Lys	Cys	Leu	Ala	Leu	Gly	Met	Ser	His	Asn	Ala	Ile	Arg
	130					135					140				
Phe	Gly	Arg	Met	Pro	Glu	Ala	Glu	Lys	Arg	Lys	Leu	Val	Ala	Gly	Leu
145					150					155					160
Thr	Ala	Asn	Glu	Gly	Ser	Gln	Tyr	Asn	Pro	Gln	Val	Ala	Asp	Leu	Lys
				165					170					175	
Ala	Phe	Ser	Lys	His	Ile	Tyr	Asn	Ala	Tyr	Leu	Lys	Asn	Phe	Asn	Met
			180					185					190		
Thr	Lys	Lys	Lys	Ala	Arg	Ser	Ile	Leu	Thr	Gly	Lys	Ala	Ser	His	Thr
		195					200					205			
Ala	Pro	Phe	Val	Ile	His	Asp	Ile	Glu	Thr	Leu	Trp	Gln	Ala	Glu	Lys
	210					215					220				
Gly	Leu	Val	Trp	Lys	Gln	Leu	Val	Asn	Gly	Leu	Pro	Pro	Tyr	Lys	Glu
225					230					235					240
Ile	Ser	Val	His	Val	Phe	Tyr	Arg	Cys	Gln	Cys	Thr	Thr	Val	Glu	Thr
				245					250					255	
Val	Arg	Glu	Leu	Thr	Glu	Phe	Ala	Lys	Ser	Ile	Pro	Ser	Phe	Ser	Ser
			260					265					270		
Leu	Phe	Leu	Asn	Asp	Gln	Val	Thr	Leu	Leu	Lys	Tyr	Gly	Val	His	Glu
	275						280					285			
Ala	Ile	Phe	Ala	Met	Leu	Ala	Ser	Ile	Val	Asn	Lys	Asp	Gly	Leu	Leu
	290					295					300				
Val	Ala	Asn	Gly	Ser	Gly	Phe	Val	Thr	Arg	Glu	Phe	Leu	Arg	Ser	Leu
305					310					315					320
Arg	Lys	Pro	Phe	Ser	Asp	Ile	Ile	Glu	Pro	Lys	Phe	Glu	Phe	Ala	Val
				325					330					335	
Lys	Phe	Asn	Ala	Leu	Glu	Leu	Asp	Asp	Ser	Asp	Leu	Ala	Leu	Phe	Ile
			340					345					350		
Ala	Ala	Ile	Ile	Leu	Cys	Gly	Asp	Arg	Pro	Gly	Leu	Met	Asn	Val	Pro
		355					360					365			
Arg	Val	Glu	Ala	Ile	Gln	Asp	Thr	Ile	Leu	Arg	Ala	Leu	Glu	Phe	His
	370					375					380				
Leu	Gln	Ala	Asn	His	Pro	Asp	Ala	Gln	Tyr	Leu	Phe	Pro	Lys	Leu	Leu







<210> 11  
 <211> 609  
 <212> PRT  
 <213> Homo sapiens

<220>  
 <221> DOMAIN  
 <222> (295)..(585)  
 <223> minimal ligand binding domain

<400> 11

Met	Asp	Thr	Glu	Asp	Leu	Pro	Ala	Asn	Asn	Ala	Pro	Leu	Thr	Val	Asn	1	5	10	15
Glu	Gln	Leu	Leu	Gly	Ser	Cys	Thr	Leu	Lys	Phe	Pro	Ala	Gln	Asp	Ala	20	25	30	
Gln	Val	Ile	Val	Met	Ser	Gly	Gln	Glu	Thr	Ile	Arg	Val	Leu	Glu	Val	35	40	45	
Glu	Val	Asp	Thr	Ala	Leu	Ser	Ser	Ala	Gly	Ala	Ala	Glu	Ser	Gly	Gly	50	55	60	
Asp	Glu	Glu	Gly	Ser	Gly	Gln	Ser	Leu	Glu	Ala	Thr	Glu	Glu	Ala	Gln	65	70	75	80
Leu	Asp	Gly	Pro	Val	Thr	Thr	Ser	Ser	Thr	Thr	Ala	Val	Thr	Val	Glu	85	90	95	
Val	Ser	Ala	Pro	Val	Val	Gln	Thr	Val	Val	Ser	Lys	Ala	Ala	Ile	Ser	100	105	110	
Val	Ser	Pro	Ala	Gln	Gln	Thr	Ser	Val	Pro	Ile	Thr	Val	Gln	Ala	Cys	115	120	125	
Pro	Gln	Val	Leu	Thr	Gln	Asp	Gly	Leu	Ala	Ser	Leu	Met	Thr	Gly	Met	130	135	140	
Leu	Ala	Gln	Gln	Ser	Ser	Leu	Gly	Gln	Pro	Leu	Leu	Ile	Pro	Leu	Ser	145	150	155	160
Met	Ala	Gly	Ser	Val	Gly	Gly	Gln	Gly	Gly	Leu	Ala	Val	Leu	Thr	Leu	165	170	175	
Pro	Thr	Ala	Thr	Val	Ala	Thr	Leu	Pro	Gly	Leu	Ala	Ala	Ala	Ser	Pro	180	185	190	
Ala	Gly	Gly	Leu	Leu	Lys	Leu	Pro	Phe	Ala	Gly	Leu	Gln	Ala	Ala	Thr	195	200	205	
Val	Leu	Asn	Ser	Val	Gln	Thr	Gln	Leu	Gln	Ala	Pro	Ala	Gln	Ala	Val	210	215	220	
Leu	Gln	Pro	Gln	Met	Ser	Ala	Leu	Ala	Met	Gln	Gln	Thr	Gln	Thr	Thr	225	230	235	240

Ala Ala Thr Thr Ala Ser Ile Val Gln Lys Ala Ser Glu Pro Ser Val  
 245 250 255  
 Ser Val Ala Thr Leu Gln Thr Ala Gly Leu Ser Ile Asn Pro Ala Ile  
 260 265 270  
 Ile Ser Ala Ala Ser Leu Gly Ala Gln Pro Gln Phe Ile Ser Ser Leu  
 275 280 285  
 Thr Thr Thr Pro Ile Ile Thr Ser Ala Met Ser Asn Val Ala Gly Leu  
 290 295 300  
 Thr Ser Gln Leu Ile Thr Asn Ala Gln Gly Gln Val Ile Gly Thr Leu  
 305 310 315 320  
 Pro Leu Leu Val Asn Pro Ala Ser Leu Ala Gly Ala Ala Ala Ala Ser  
 325 330 335  
 Ala Leu Pro Ala Gln Gly Leu Gln Val Gln Thr Val Ala Pro Gln Leu  
 340 345 350  
 Leu Leu Asn Ser Gln Gly Gln Ile Ile Ala Thr Ile Gly Asn Gly Pro  
 355 360 365  
 Thr Ala Ala Ile Pro Ser Thr Ala Ser Val Leu Pro Lys Ala Thr Val  
 370 375 380  
 Pro Leu Thr Leu Thr Lys Thr Thr Thr Gln Gly Pro Val Gly Lys Val  
 385 390 395 400  
 Ala Pro Ser Lys Val Ile Ile Ala Pro Gln Pro Ser Val Val Lys Pro  
 405 410 415  
 Val Thr Ser Leu Thr Ala Ala Gly Val Ile Ala Cys Gly Glu Met Pro  
 420 425 430  
 Thr Val Gly Gln Leu Val Asn Lys Pro Ser Ala Val Lys Asp Glu Glu  
 435 440 445  
 Ala Ile Asn Leu Glu Glu Ile Arg Glu Phe Ala Lys Asn Phe Lys Ile  
 450 455 460  
 Arg Arg Leu Ser Leu Gly Leu Thr Gln Thr Gln Val Gly Gln Ala Leu  
 465 470 475 480  
 Thr Ala Thr Glu Gly Pro Ala Tyr Ser Gln Ser Ala Ile Cys Arg Phe  
 485 490 495  
 Glu Lys Leu Asp Ile Thr Pro Lys Ser Ala Gln Lys Leu Lys Pro Val  
 500 505 510  
 Leu Glu Arg Trp Leu Ala Glu Ala Glu Leu Trp Asn Gln Lys Gly Gln  
 515 520 525  
 Gln Asn Leu Met Glu Phe Val Gly Gly Glu Pro Ser Lys Lys Arg Lys  
 530 535 540

Arg Arg Thr Ser Phe Thr Pro Gln Ala Ile Glu Val Leu Asn Thr Tyr  
545 550 555 560

Phe Glu Lys Asn Ser Leu Pro Thr Gly Gln Glu Ile Thr Glu Ile Ala  
565 570 575

Lys Glu Leu Asn Tyr Asp Arg Glu Val Val Arg Val Trp Phe Cys Asn  
580 585 590

Arg Arg Gln Thr Leu Lys Asn Thr Ser Lys Ile Asn Val Phe Gln Ser  
595 600 605

Gln

<210> 12  
<211> 595  
<212> PRT  
<213> Homo sapiens

<220>  
<221> DOMAIN  
<222> (287)..(549)  
<223> minimal ligand binding domain

<400> 12

Met Thr Met Thr Leu His Thr Lys Ala Ser Gly Met Ala Leu Leu His  
1 5 10 15

Gln Ile Gln Gly Asn Glu Leu Glu Pro Leu Asn Arg Pro Gln Leu Lys  
20 25 30

Ile Pro Leu Glu Arg Pro Leu Gly Glu Val Tyr Leu Asp Ser Ser Lys  
35 40 45

Pro Ala Val Tyr Asn Tyr Pro Glu Gly Ala Ala Tyr Glu Phe Asn Ala  
50 55 60

Ala Ala Ala Ala Asn Ala Gln Val Tyr Gly Gln Thr Gly Leu Pro Tyr  
65 70 75 80

Gly Pro Gly Ser Glu Ala Ala Ala Phe Gly Ser Asn Gly Leu Gly Gly  
85 90 95

Phe Pro Pro Leu Asn Ser Val Ser Pro Ser Pro Leu Met Leu Leu His  
100 105 110

Pro Pro Pro Gln Leu Ser Pro Phe Leu Gln Pro His Gly Gln Gln Val  
115 120 125

Pro Tyr Tyr Leu Glu Asn Glu Pro Ser Gly Tyr Thr Val Arg Glu Ala  
130 135 140

Gly Pro Pro Ala Phe Tyr Arg Pro Asn Ser Asp Asn Arg Arg Gln Gly

145					150						155				160
Gly	Arg	Glu	Arg	Leu	Ala	Ser	Thr	Asn	Asp	Lys	Gly	Ser	Met	Ala	Met
				165					170					175	
Glu	Ser	Ala	Lys	Glu	Thr	Arg	Tyr	Cys	Ala	Val	Cys	Asn	Asp	Tyr	Ala
			180					185					190		
Ser	Gly	Tyr	His	Tyr	Gly	Val	Trp	Ser	Cys	Glu	Gly	Cys	Lys	Ala	Phe
		195					200					205			
Phe	Lys	Arg	Ser	Ile	Gln	Gly	His	Asn	Asp	Tyr	Met	Cys	Pro	Ala	Thr
	210					215					220				
Asn	Gln	Cys	Thr	Ile	Asp	Lys	Asn	Arg	Arg	Lys	Ser	Cys	Gln	Ala	Cys
225					230					235					240
Arg	Leu	Arg	Lys	Cys	Tyr	Glu	Val	Gly	Met	Met	Lys	Gly	Gly	Ile	Arg
				245					250					255	
Lys	Asp	Arg	Arg	Gly	Gly	Arg	Met	Leu	Lys	His	Lys	Arg	Gln	Arg	Asp
			260					265					270		
Asp	Gly	Glu	Gly	Arg	Gly	Glu	Val	Gly	Ser	Ala	Gly	Asp	Met	Arg	Ala
		275					280					285			
Ala	Asn	Leu	Trp	Pro	Ser	Pro	Leu	Met	Ile	Lys	Arg	Ser	Lys	Lys	Asn
	290					295				300					
Ser	Leu	Ala	Leu	Ser	Leu	Thr	Ala	Asp	Gln	Met	Val	Ser	Ala	Leu	Leu
305					310					315					320
Asp	Ala	Glu	Pro	Pro	Ile	Leu	Tyr	Ser	Glu	Tyr	Asp	Pro	Thr	Arg	Pro
				325					330					335	
Phe	Ser	Glu	Ala	Ser	Met	Met	Gly	Leu	Leu	Thr	Asn	Leu	Ala	Asp	Arg
			340					345					350		
Glu	Leu	Val	His	Met	Ile	Asn	Trp	Ala	Lys	Arg	Val	Pro	Gly	Phe	Val
		355					360					365			
Asp	Leu	Thr	Leu	His	Asp	Gln	Val	His	Leu	Leu	Glu	Cys	Ala	Trp	Leu
	370					375					380				
Glu	Ile	Leu	Met	Ile	Gly	Leu	Val	Trp	Arg	Ser	Met	Glu	His	Pro	Gly
385					390					395					400
Lys	Leu	Leu	Phe	Ala	Pro	Asn	Leu	Leu	Leu	Asp	Arg	Asn	Gln	Gly	Lys
			405					410						415	
Cys	Val	Glu	Gly	Met	Val	Glu	Ile	Phe	Asp	Met	Leu	Leu	Ala	Thr	Ser
			420					425					430		
Ser	Arg	Phe	Arg	Met	Met	Asn	Leu	Gln	Gly	Glu	Glu	Phe	Val	Cys	Leu
		435					440					445			
Lys	Ser	Ile	Ile	Leu	Leu	Asn	Ser	Gly	Val	Tyr	Thr	Phe	Leu	Ser	Ser

450		455		460
Thr Leu Lys Ser Leu Glu Glu Lys Asp His Ile His Arg Val Leu Asp				
465		470		480
Lys Ile Thr Asp Thr Leu Ile His Leu Met Ala Lys Ala Gly Leu Thr				
	485		490	495
Leu Gln Gln Gln His Gln Arg Leu Ala Gln Leu Leu Leu Ile Leu Ser				
	500		505	510
His Ile Arg His Met Ser Asn Lys Gly Met Glu His Leu Tyr Ser Met				
	515		520	525
Lys Cys Lys Asn Val Val Pro Leu Tyr Asp Leu Leu Leu Glu Met Leu				
	530		535	540
Asp Ala His Arg Leu His Ala Pro Thr Ser Arg Gly Gly Ala Ser Val				
545		550		560
Glu Glu Thr Asp Gln Ser His Leu Ala Thr Ala Gly Ser Thr Ser Ser				
	565		570	575
His Ser Leu Gln Lys Tyr Tyr Ile Thr Gly Glu Ala Glu Gly Phe Pro				
	580		585	590

Ala Thr Val  
595

<210> 13  
 <211> 777  
 <212> PRT  
 <213> Homo sapiens  
  
 <220>  
 <221> DOMAIN  
 <222> (506)..(762)  
 <223> minimal ligand binding domain

<400> 13

Met Asp Ser Lys Glu Ser Leu Thr Pro Gly Arg Glu Glu Asn Pro Ser				
1		5		10
Ser Val Leu Ala Gln Glu Arg Gly Asp Val Met Asp Phe Tyr Lys Thr				
	20		25	30
Leu Arg Gly Gly Ala Thr Val Lys Val Ser Ala Ser Ser Pro Ser Leu				
	35		40	45
Ala Val Ala Ser Gln Ser Asp Ser Lys Gln Arg Arg Leu Leu Val Asp				
	50		55	60
Phe Pro Lys Gly Ser Val Ser Asn Ala Gln Gln Pro Asp Leu Ser Lys				
65		70		75
				80



Ala Val Ser Leu Ser Met Gly Leu Tyr Met Gly Glu Thr Glu Thr Lys  
                             85                            90                            95  
 Val Met Gly Asn Asp Leu Gly Phe Pro Gln Gln Gly Gln Ile Ser Leu  
                             100                            105                            110  
 Ser Ser Gly Glu Thr Asp Leu Lys Leu Leu Glu Glu Ser Ile Ala Asn  
                             115                            120                            125  
 Leu Asn Arg Ser Thr Ser Val Pro Glu Asn Pro Lys Ser Ser Ala Ser  
                             130                            135                            140  
 Thr Ala Val Ser Ala Ala Pro Thr Glu Lys Glu Phe Pro Lys Thr His  
 145                            150                            155                            160  
 Ser Asp Val Ser Ser Glu Gln Gln His Leu Lys Gly Gln Thr Gly Thr  
                             165                            170                            175  
 Asn Gly Gly Asn Val Lys Leu Tyr Thr Thr Asp Gln Ser Thr Phe Asp  
                             180                            185                            190  
 Ile Leu Gln Asp Leu Glu Phe Ser Ser Gly Ser Pro Gly Lys Glu Thr  
                             195                            200                            205  
 Asn Glu Ser Pro Trp Arg Ser Asp Leu Leu Ile Asp Glu Asn Cys Leu  
                             210                            215                            220  
 Leu Ser Pro Leu Ala Gly Glu Asp Asp Ser Phe Leu Leu Glu Gly Asn  
 225                            230                            235                            240  
 Ser Asn Glu Asp Cys Lys Pro Leu Ile Leu Pro Asp Thr Lys Pro Lys  
                             245                            250                            255  
 Ile Lys Asp Asn Gly Asp Leu Val Leu Ser Ser Pro Ser Asn Val Thr  
                             260                            265                            270  
 Leu Pro Gln Val Lys Thr Glu Lys Glu Asp Phe Ile Glu Leu Cys Thr  
                             275                            280                            285  
 Pro Gly Val Ile Lys Gln Glu Lys Leu Gly Thr Val Tyr Cys Gln Ala  
                             290                            295                            300  
 Ser Phe Pro Gly Ala Asn Ile Ile Gly Asn Lys Met Ser Ala Ile Ser  
 305                            310                            315                            320  
 Val His Gly Val Ser Thr Ser Gly Gly Gln Met Tyr His Tyr Asp Met  
                             325                            330                            335  
 Asn Thr Ala Ser Leu Ser Gln Gln Gln Asp Gln Lys Pro Ile Phe Asn  
                             340                            345                            350  
 Val Ile Pro Pro Ile Pro Val Gly Ser Glu Asn Trp Asn Arg Cys Gln  
                             355                            360                            365  
 Gly Ser Gly Asp Asp Asn Leu Thr Ser Leu Gly Thr Leu Asn Phe Pro  
                             370                            375                            380

Gly	Arg	Thr	Val	Phe	Ser	Asn	Gly	Tyr	Ser	Ser	Pro	Ser	Met	Arg	Pro	385	390	395	400
Asp	Val	Ser	Ser	Pro	Pro	Ser	Ser	Ser	Ser	Thr	Ala	Thr	Thr	Gly	Pro	405	410	415	
Pro	Pro	Lys	Leu	Cys	Leu	Val	Cys	Ser	Asp	Glu	Ala	Ser	Gly	Cys	His	420	425	430	
Tyr	Gly	Val	Leu	Thr	Cys	Gly	Ser	Cys	Lys	Val	Phe	Phe	Lys	Arg	Ala	435	440	445	
Val	Glu	Gly	Gln	His	Asn	Tyr	Leu	Cys	Ala	Gly	Arg	Asn	Asp	Cys	Ile	450	455	460	
Ile	Asp	Lys	Ile	Arg	Arg	Lys	Asn	Cys	Pro	Ala	Cys	Arg	Tyr	Arg	Lys	465	470	475	480
Cys	Leu	Gln	Ala	Gly	Met	Asn	Leu	Glu	Ala	Arg	Lys	Thr	Lys	Lys	Lys	485	490	495	
Ile	Lys	Gly	Ile	Gln	Gln	Ala	Thr	Thr	Gly	Val	Ser	Gln	Glu	Thr	Ser	500	505	510	
Glu	Asn	Pro	Gly	Asn	Lys	Thr	Ile	Val	Pro	Ala	Thr	Leu	Pro	Gln	Leu	515	520	525	
Thr	Pro	Thr	Leu	Val	Ser	Leu	Leu	Glu	Val	Ile	Glu	Pro	Glu	Val	Leu	530	535	540	
Tyr	Ala	Gly	Tyr	Asp	Ser	Ser	Val	Pro	Asp	Ser	Thr	Trp	Arg	Ile	Met	545	550	555	560
Thr	Thr	Leu	Asn	Met	Leu	Gly	Gly	Arg	Gln	Val	Ile	Ala	Ala	Val	Lys	565	570	575	
Trp	Ala	Lys	Ala	Ile	Pro	Gly	Phe	Arg	Asn	Leu	His	Leu	Asp	Asp	Gln	580	585	590	
Met	Thr	Leu	Leu	Gln	Tyr	Ser	Trp	Met	Phe	Leu	Met	Ala	Phe	Ala	Leu	595	600	605	
Gly	Trp	Arg	Ser	Tyr	Arg	Gln	Ser	Ser	Ala	Asn	Leu	Leu	Cys	Phe	Ala	610	615	620	
Pro	Asp	Leu	Ile	Ile	Asn	Glu	Gln	Arg	Met	Thr	Leu	Pro	Cys	Met	Tyr	625	630	635	640
Asp	Gln	Cys	Lys	His	Met	Leu	Tyr	Val	Ser	Ser	Glu	Leu	His	Arg	Leu	645	650	655	
Gln	Val	Ser	Tyr	Glu	Glu	Tyr	Leu	Cys	Met	Lys	Thr	Leu	Leu	Leu	Leu	660	665	670	
Ser	Ser	Val	Pro	Lys	Asp	Gly	Leu	Lys	Ser	Gln	Glu	Leu	Phe	Asp	Glu	675	680	685	

Ile Arg Met Thr Tyr Ile Lys Glu Leu Gly Lys Ala Ile Val Lys Arg  
690 695 700

Glu Gly Asn Ser Ser Gln Asn Trp Gln Arg Phe Tyr Gln Leu Thr Lys  
705 710 715 720

Leu Leu Asp Ser Met His Glu Val Val Glu Asn Leu Leu Asn Tyr Cys  
725 730 735

Phe Gln Thr Phe Leu Asp Lys Thr Met Ser Ile Glu Phe Pro Glu Met  
740 745 750

Leu Ala Glu Ile Ile Thr Asn Gln Ile Pro Lys Tyr Ser Asn Gly Asn  
755 760 765

Ile Lys Lys Leu Leu Phe His Gln Lys  
770 775

<210> 14

<211> 933

<212> PRT

<213> Homo sapiens

<220>

<221> DOMAIN

<222> (659)..(918)

<223> minimal ligand binding domain

<400> 14

Met Thr Glu Leu Lys Ala Lys Gly Pro Arg Ala Pro His Val Ala Gly  
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Gly Pro Pro Ser Pro Glu Val Gly Ser Pro Leu Leu Cys Arg Pro Ala  
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Ala Gly Pro Phe Pro Gly Ser Gln Thr Ser Asp Thr Leu Pro Glu Val  
35 40 45

Ser Ala Ile Pro Ile Ser Leu Asp Gly Leu Leu Phe Pro Arg Pro Cys  
50 55 60

Gln Gly Gln Asp Pro Ser Asp Glu Lys Thr Gln Asp Gln Gln Ser Leu  
65 70 75 80

Ser Asp Val Glu Gly Ala Tyr Ser Arg Ala Glu Ala Thr Arg Gly Ala  
85 90 95

Gly Gly Ser Ser Ser Ser Pro Pro Glu Lys Asp Ser Gly Leu Leu Asp  
100 105 110

Ser Val Leu Asp Thr Leu Leu Ala Pro Ser Gly Pro Gly Gln Ser Gln  
115 120 125

Pro Ser Pro Pro Ala Cys Glu Val Thr Ser Ser Trp Cys Leu Phe Gly  
130 135 140

Pro Glu Leu Pro Glu Asp Pro Pro Ala Ala Pro Ala Thr Gln Arg Val  
 145 150 155 160  
 Leu Ser Pro Leu Met Ser Arg Ser Gly Cys Lys Val Gly Asp Ser Ser  
 165 170 175  
 Gly Thr Ala Ala Ala His Lys Val Leu Pro Arg Gly Leu Ser Pro Ala  
 180 185 190  
 Arg Gln Leu Leu Leu Pro Ala Ser Glu Ser Pro His Trp Ser Gly Ala  
 195 200 205  
 Pro Val Lys Pro Ser Pro Gln Ala Ala Ala Val Glu Val Glu Glu Glu  
 210 215 220  
 Asp Ser Ser Glu Ser Glu Glu Ser Ala Gly Pro Leu Leu Lys Gly Lys  
 225 230 235 240  
 Pro Arg Ala Leu Gly Gly Ala Ala Ala Gly Gly Gly Ala Ala Ala Cys  
 245 250 255  
 Pro Pro Gly Ala Ala Ala Gly Gly Val Ala Leu Val Pro Lys Glu Asp  
 260 265 270  
 Ser Arg Phe Ser Ala Pro Arg Val Ala Leu Val Glu Gln Asp Ala Pro  
 275 280 285  
 Met Ala Pro Gly Arg Ser Pro Leu Ala Thr Thr Val Met Asp Phe Ile  
 290 295 300  
 His Val Pro Ile Leu Pro Leu Asn His Ala Leu Leu Ala Ala Arg Thr  
 305 310 315 320  
 Arg Gln Leu Leu Glu Asp Glu Ser Tyr Asp Gly Gly Ala Gly Ala Ala  
 325 330 335  
 Ser Ala Phe Ala Pro Pro Arg Thr Ser Pro Cys Ala Ser Ser Thr Pro  
 340 345 350  
 Val Ala Val Gly Asp Phe Pro Asp Cys Ala Tyr Pro Pro Asp Ala Glu  
 355 360 365  
 Pro Lys Asp Asp Ala Tyr Pro Leu Tyr Ser Asp Phe Gln Pro Pro Ala  
 370 375 380  
 Leu Lys Ile Lys Glu Glu Glu Glu Gly Ala Glu Ala Ser Ala Arg Ser  
 385 390 395 400  
 Pro Arg Ser Tyr Leu Val Ala Gly Ala Asn Pro Ala Ala Phe Pro Asp  
 405 410 415  
 Phe Pro Leu Gly Pro Pro Pro Pro Leu Pro Pro Arg Ala Thr Pro Ser  
 420 425 430  
 Arg Pro Gly Glu Ala Ala Val Thr Ala Ala Pro Ala Ser Ala Ser Val  
 435 440 445

Ser Ser Ala Ser Ser Ser Gly Ser Thr Leu Glu Cys Ile Leu Tyr Lys  
 450 455 460  
 Ala Glu Gly Ala Pro Pro Gln Gln Gly Pro Phe Ala Pro Pro Pro Cys  
 465 470 475 480  
 Lys Ala Pro Gly Ala Ser Gly Cys Leu Leu Pro Arg Asp Gly Leu Pro  
 485 490 495  
 Ser Thr Ser Ala Ser Ala Ala Ala Gly Ala Ala Pro Ala Leu Tyr  
 500 505 510  
 Pro Ala Leu Gly Leu Asn Gly Leu Pro Gln Leu Gly Tyr Gln Ala Ala  
 515 520 525  
 Val Leu Lys Glu Gly Leu Pro Gln Val Tyr Pro Pro Tyr Leu Asn Tyr  
 530 535 540  
 Leu Arg Pro Asp Ser Glu Ala Ser Gln Ser Pro Gln Tyr Ser Phe Glu  
 545 550 555 560  
 Ser Leu Pro Gln Lys Ile Cys Leu Ile Cys Gly Asp Glu Ala Ser Gly  
 565 570 575  
 Cys His Tyr Gly Val Leu Thr Cys Gly Ser Cys Lys Val Phe Phe Lys  
 580 585 590  
 Arg Ala Met Glu Gly Gln His Asn Tyr Leu Cys Ala Gly Arg Asn Asp  
 595 600 605  
 Cys Ile Val Asp Lys Ile Arg Arg Lys Asn Cys Pro Ala Cys Arg Leu  
 610 615 620  
 Arg Lys Cys Cys Gln Ala Gly Met Val Leu Gly Gly Arg Lys Phe Lys  
 625 630 635 640  
 Lys Phe Asn Lys Val Arg Val Val Arg Ala Leu Asp Ala Val Ala Leu  
 645 650 655  
 Pro Gln Pro Leu Gly Val Pro Asn Glu Ser Gln Ala Leu Ser Gln Arg  
 660 665 670  
 Phe Thr Phe Ser Pro Gly Gln Asp Ile Gln Leu Ile Pro Pro Leu Ile  
 675 680 685  
 Asn Leu Leu Met Ser Ile Glu Pro Asp Val Ile Tyr Ala Gly His Asp  
 690 695 700  
 Asn Thr Lys Pro Asp Thr Ser Ser Ser Leu Leu Thr Ser Leu Asn Gln  
 705 710 715 720  
 Leu Gly Glu Arg Gln Leu Leu Ser Val Val Lys Trp Ser Lys Ser Leu  
 725 730 735  
 Pro Gly Phe Arg Asn Leu His Ile Asp Asp Gln Ile Thr Leu Ile Gln  
 740 745 750



Tyr Ser Trp Met Ser Leu Met Val Phe Gly Leu Gly Trp Arg Ser Tyr  
755 760 765

Lys His Val Ser Gly Gln Met Leu Tyr Phe Ala Pro Asp Leu Ile Leu  
770 775 780

Asn Glu Gln Arg Met Lys Glu Ser Ser Phe Tyr Ser Leu Cys Leu Thr  
785 790 795 800

Met Trp Gln Ile Pro Gln Glu Phe Val Lys Leu Gln Val Ser Gln Glu  
805 810 815

Glu Phe Leu Cys Met Lys Val Leu Leu Leu Asn Thr Ile Pro Leu  
820 825 830

Glu Gly Leu Arg Ser Gln Thr Gln Phe Glu Glu Met Arg Ser Ser Tyr  
835 840 845

Ile Arg Glu Leu Ile Lys Ala Ile Gly Leu Arg Gln Lys Gly Val Val  
850 855 860

Ser Ser Ser Gln Arg Phe Tyr Gln Leu Thr Lys Leu Leu Asp Asn Leu  
865 870 875 880

His Asp Leu Val Lys Gln Leu His Leu Tyr Cys Leu Asn Thr Phe Ile  
885 890 895

Gln Ser Arg Ala Leu Ser Val Glu Phe Pro Glu Met Met Ser Glu Val  
900 905 910

Ile Ala Ala Gln Leu Pro Lys Ile Leu Ala Gly Met Val Lys Pro Leu  
915 920 925

Leu Phe His Lys Lys  
930

<210> 15  
<211> 984  
<212> PRT  
<213> Homo sapiens

<220>  
<221> DOMAIN  
<222> (695)..(969)  
<223> minimal ligand binding domain

<400> 15

Met Glu Thr Lys Gly Tyr His Ser Leu Pro Glu Gly Leu Asp Met Glu  
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Arg Arg Trp Gly Gln Val Ser Gln Ala Val Glu Arg Ser Ser Leu Gly  
20 25 30

Pro Thr Glu Arg Thr Asp Glu Asn Asn Tyr Met Glu Ile Val Asn Val



	340		345		350														
Ser	Thr	Leu	Arg	Asp	Val	Val	Pro	Ser	Pro	Asp	Thr	Gln	Glu	Lys	Gly				
		355					360					365							
Ala	Gln	Glu	Val	Pro	Phe	Pro	Lys	Thr	Glu	Glu	Val	Glu	Ser	Ala	Ile				
	370					375					380								
Ser	Asn	Gly	Val	Thr	Gly	Gln	Leu	Asn	Ile	Val	Gln	Tyr	Ile	Lys	Pro				
385					390					395					400				
Glu	Pro	Asp	Gly	Ala	Phe	Ser	Ser	Ser	Cys	Leu	Gly	Gly	Asn	Ser	Lys				
				405					410					415					
Ile	Asn	Ser	Asp	Ser	Ser	Phe	Ser	Val	Pro	Ile	Lys	Gln	Glu	Ser	Thr				
			420					425					430						
Lys	His	Ser	Cys	Ser	Gly	Thr	Ser	Phe	Lys	Gly	Asn	Pro	Thr	Val	Asn				
		435					440					445							
Pro	Phe	Pro	Phe	Met	Asp	Gly	Ser	Tyr	Phe	Ser	Phe	Met	Asp	Asp	Lys				
	450					455					460								
Asp	Tyr	Tyr	Ser	Leu	Ser	Gly	Ile	Leu	Gly	Pro	Pro	Val	Pro	Gly	Phe				
465					470				475					480					
Asp	Gly	Asn	Cys	Glu	Gly	Ser	Gly	Phe	Pro	Val	Gly	Ile	Lys	Gln	Glu				
				485				490						495					
Pro	Asp	Asp	Gly	Ser	Tyr	Tyr	Pro	Glu	Ala	Ser	Ile	Pro	Ser	Ser	Ala				
			500					505				510							
Ile	Val	Gly	Val	Asn	Ser	Gly	Gly	Gln	Ser	Phe	His	Tyr	Arg	Ile	Gly				
		515					520					525							
Ala	Gln	Gly	Thr	Ile	Ser	Leu	Ser	Arg	Ser	Ala	Arg	Asp	Gln	Ser	Phe				
	530					535				540									
Gln	His	Leu	Ser	Ser	Phe	Pro	Pro	Val	Asn	Thr	Leu	Val	Glu	Ser	Trp				
545					550					555					560				
Lys	Ser	His	Gly	Asp	Leu	Ser	Ser	Arg	Arg	Ser	Asp	Gly	Tyr	Pro	Val				
				565				570						575					
Leu	Glu	Tyr	Ile	Pro	Glu	Asn	Val	Ser	Ser	Ser	Thr	Leu	Arg	Ser	Val				
			580					585					590						
Ser	Thr	Gly	Ser	Ser	Arg	Pro	Ser	Lys	Ile	Cys	Leu	Val	Cys	Gly	Asp				
		595					600					605							
Glu	Ala	Ser	Gly	Cys	His	Tyr	Gly	Val	Val	Thr	Cys	Gly	Ser	Cys	Lys				
	610					615				620									
Val	Phe	Phe	Lys	Arg	Ala	Val	Glu	Gly	Gln	His	Asn	Tyr	Leu	Cys	Ala				
625					630					635					640				
Gly	Arg	Asn	Asp	Cys	Ile	Ile	Asp	Lys	Ile	Arg	Arg	Lys	Asn	Cys	Pro				

645					650					655						
Ala	Cys	Arg	Leu	Gln	Lys	Cys	Leu	Gln	Ala	Gly	Met	Asn	Leu	Gly	Ala	
660					665					670						
Arg	Lys	Ser	Lys	Lys	Leu	Gly	Lys	Leu	Lys	Gly	Ile	His	Glu	Glu	Gln	
675					680					685						
Pro	Gln	Gln	Gln	Gln	Pro	Pro	Pro	Pro	Pro	Pro	Pro	Pro	Gln	Ser	Pro	
690					695					700						
Glu	Glu	Gly	Thr	Thr	Tyr	Ile	Ala	Pro	Ala	Lys	Glu	Pro	Ser	Val	Asn	
705					710					715					720	
Thr	Ala	Leu	Val	Pro	Gln	Leu	Ser	Thr	Ile	Ser	Arg	Ala	Leu	Thr	Pro	
725					730					735						
Ser	Pro	Val	Met	Val	Leu	Glu	Asn	Ile	Glu	Pro	Glu	Ile	Val	Tyr	Ala	
740					745					750						
Gly	Tyr	Asp	Ser	Ser	Lys	Pro	Asp	Thr	Ala	Glu	Asn	Leu	Leu	Ser	Thr	
755					760					765						
Leu	Asn	Arg	Leu	Ala	Gly	Lys	Gln	Met	Ile	Gln	Val	Val	Lys	Trp	Ala	
770					775					780						
Lys	Val	Leu	Pro	Gly	Phe	Lys	Asn	Leu	Pro	Leu	Glu	Asp	Gln	Ile	Thr	
785					790					795					800	
Leu	Ile	Gln	Tyr	Ser	Trp	Met	Cys	Leu	Ser	Ser	Phe	Ala	Leu	Ser	Trp	
805					810					815						
Arg	Ser	Tyr	Lys	His	Thr	Asn	Ser	Gln	Phe	Leu	Tyr	Phe	Ala	Pro	Asp	
820					825					830						
Leu	Val	Phe	Asn	Glu	Glu	Lys	Met	His	Gln	Ser	Ala	Met	Tyr	Glu	Leu	
835					840					845						
Cys	Gln	Gly	Met	His	Gln	Ile	Ser	Leu	Gln	Phe	Val	Arg	Leu	Gln	Leu	
850					855					860						
Thr	Phe	Glu	Glu	Tyr	Thr	Ile	Met	Lys	Val	Leu	Leu	Leu	Leu	Ser	Thr	
865					870					875					880	
Ile	Pro	Lys	Asp	Gly	Leu	Lys	Ser	Gln	Ala	Ala	Phe	Glu	Glu	Met	Arg	
885					890					895						
Thr	Asn	Tyr	Ile	Lys	Glu	Leu	Arg	Lys	Met	Val	Thr	Lys	Cys	Pro	Asn	
900					905					910						
Asn	Ser	Gly	Gln	Ser	Trp	Gln	Arg	Phe	Tyr	Gln	Leu	Thr	Lys	Leu	Leu	
915					920					925						
Asp	Ser	Met	His	Asp	Leu	Val	Ser	Asp	Leu	Leu	Glu	Phe	Cys	Phe	Tyr	
930					935					940						
Thr	Phe	Arg	Glu	Ser	His	Ala	Leu	Lys	Val	Glu	Phe	Pro	Ala	Met	Leu	





Thr	Val	Ser	His	Ile	Glu	Gly	Tyr	Glu	Cys	Gln	Pro	Ile	Phe	Leu	Asn	
		195					200					205				
Val	Leu	Glu	Ala	Ile	Glu	Pro	Gly	Val	Val	Cys	Ala	Gly	His	Asp	Asn	
	210					215					220					
Asn	Gln	Pro	Asp	Ser	Phe	Ala	Ala	Leu	Leu	Ser	Ser	Leu	Asn	Glu	Leu	
225					230					235					240	
Gly	Glu	Arg	Gln	Leu	Val	His	Val	Val	Lys	Trp	Ala	Lys	Ala	Leu	Pro	
				245					250					255		
Gly	Phe	Arg	Asn	Leu	His	Val	Asp	Asp	Gln	Met	Ala	Val	Ile	Gln	Tyr	
			260					265					270			
Ser	Trp	Met	Gly	Leu	Met	Val	Phe	Ala	Met	Gly	Trp	Arg	Ser	Phe	Thr	
		275					280					285				
Asn	Val	Asn	Ser	Arg	Met	Leu	Tyr	Phe	Ala	Pro	Asp	Leu	Val	Phe	Asn	
	290					295					300					
Glu	Tyr	Arg	Met	His	Lys	Ser	Arg	Met	Tyr	Ser	Gln	Cys	Val	Arg	Met	
305					310					315					320	
Arg	His	Leu	Ser	Gln	Glu	Phe	Gly	Trp	Leu	Gln	Ile	Thr	Pro	Gln	Glu	
				325					330					335		
Phe	Leu	Cys	Met	Lys	Ala	Leu	Leu	Leu	Phe	Ser	Ile	Ile	Pro	Val	Asp	
			340					345					350			
Gly	Leu	Lys	Asn	Gln	Lys	Phe	Phe	Asp	Glu	Leu	Arg	Met	Asn	Tyr	Ile	
		355					360					365				
Lys	Glu	Leu	Asp	Arg	Ile	Ile	Ala	Cys	Lys	Arg	Lys	Asn	Pro	Thr	Ser	
	370					375					380					
Cys	Ser	Arg	Arg	Phe	Tyr	Gln	Leu	Thr	Lys	Leu	Leu	Asp	Ser	Val	Gln	
385					390					395					400	
Pro	Ile	Ala	Arg	Glu	Leu	His	Gln	Phe	Thr	Phe	Asp	Leu	Leu	Ile	Lys	
				405					410					415		
Ser	His	Met	Val	Ser	Val	Asp	Phe	Pro	Glu	Met	Met	Ala	Glu	Ile	Ile	
			420					425					430			
Ser	Val	Gln	Val	Pro	Lys	Ile	Leu	Ser	Gly	Lys	Val	Lys	Pro	Ile	Tyr	
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Phe	His	Thr	Gln													
	450															

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 <212> DNA  
 <213> Artificial/Unknown

<220>

